Supporting Information "Competing, Coverage Dependent, Decomposition Pathways for C_2H_y Species on Nickel (111)" by Jonathan E. Mueller, Adri C. T. van Duin, and William A. Goddard III.

For each species the following information is provided in the following order as available:

- Periodic calculations:
  - # of atoms, unit cell vector lengths and angles
  - atomic coordinates (xyz format
  - total energy
  - atomic spin densities
  - atomic charges
  - atomic band centers
- Cluster calculations:
  - atomic coordinates
  - thermodynamic properties

Ni slab/clusters

Ni slab in periodic cell

24 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni	0.00000	0.00000	0.00000
Ni	0.00000	2.49184	0.00000
Ni	2.15800	1.24592	0.00000
Ni	2.15800	3.73776	0.00000
Ni	4.31600	0.00000	0.00000
Ni	4.31600	2.49184	0.00000
Ni	0.71933	1.24592	2.03458
Ni	0.71933	3.73776	2.03458
Ni	2.87733	0.00000	2.03458
Ni	2.87733	2.49184	2.03458
Ni	5.03533	1.24592	2.03458
Ni	5.03533	3.73776	2.03458
Ni	1.43855	0.00003	4.06157
Ni	1.43855	2.49187	4.06157
Ni	3.59649	1.24601	4.06179
Ni	3.59654	3.73784	4.06169
Ni	5.75432	0.00015	4.06136
Ni	5.75432	2.49200	4.06135
Ni	1.43867	0.00000	-2.03458
Ni	1.43867	2.49184	-2.03458
Ni	3.59667	1.24592	-2.03458
Ni	3.59667	3.73776	-2.03458
Ni	5.75467	0.00000	-2.03458
Ni	5.75467	2.49184	-2.03458

FINAL RELAXED ENERGY = -2246.7105256601

Total electrons from output= 240
Spin up from output= 128.5000000000
Spin down from output= 111.5000000000
Fermi level up from output= -4.9295357388
Fermi level down from output= -5.0218619832
# of atoms= 24

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 2, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 3, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 4, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 5, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 6, 0.015, -0.013, -0.012, -0.017, 0.154, 0.146, 0.146, 0.154, 0.174, 0.746
Atom 7, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.153, 0.173, 0.746
Atom 8, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.153, 0.173, 0.746
Atom 9, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.153, 0.173, 0.746
Atom 10, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.154, 0.173, 0.746
Atom 11, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.154, 0.173, 0.746
Atom 12, 0.015, -0.013, -0.012, -0.018, 0.153, 0.146, 0.147, 0.154, 0.173, 0.746
Atom 13, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 14, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 15, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 16, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 17, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 18, 0.012, -0.014, -0.016, -0.010, 0.159, 0.115, 0.110, 0.145, 0.210, 0.710
Atom 19, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
Atom 20, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
Atom 21, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
Atom 22, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
Atom 23, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
Atom 24, 0.011, -0.014, -0.016, -0.010, 0.159, 0.114, 0.109, 0.144, 0.209, 0.707
total spin= 17.4528641243215

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.706, 9.991
Atom 2, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.705, 9.991
Atom 3, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.705, 9.991
Atom 4, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.705, 9.991
Atom 5, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.706, 9.991
Atom 6, 0.271, 0.331, 0.333, 0.336, 1.745, 1.761, 1.764, 1.745, 1.705, 9.991
Atom 7, 0.268, 0.332, 0.333, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 8, 0.268, 0.332, 0.333, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 9, 0.269, 0.332, 0.333, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 10, 0.269, 0.332, 0.333, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 11, 0.268, 0.332, 0.334, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 12, 0.268, 0.332, 0.334, 0.337, 1.745, 1.760, 1.763, 1.746, 1.706, 9.992
Atom 13, 0.438, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 14, 0.438, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 15, 0.438, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 16, 0.438, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 17, 0.437, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 18, 0.437, 0.301, 0.300, 0.167, 1.728, 1.804, 1.807, 1.733, 1.705, 9.983
Atom 19, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.808, 1.733, 1.705, 9.986
Atom 20, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.808, 1.733, 1.705, 9.986
Atom 21, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.809, 1.733, 1.705, 9.986
Atom 22, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.809, 1.733, 1.705, 9.986
Atom 23, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.809, 1.733, 1.705, 9.986
Atom 24, 0.440, 0.301, 0.299, 0.167, 1.728, 1.805, 1.809, 1.733, 1.705, 9.986

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 2, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 3, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 4, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 5, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 6, -5.196, -3.925, -3.900, -4.109, -2.092, -1.833, -1.827, -2.080, -2.219, -2.219
Atom 7, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 8, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 9, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 10, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 11, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 12, -5.202, -3.938, -3.913, -4.115, -2.092, -1.859, -1.846, -2.080, -2.225, -2.225
Atom 13, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 14, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 15, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 16, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 17, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 18, -4.197, -3.205, -3.224, -1.776, -1.922, -1.511, -1.505, -1.909, -1.631, -1.732
Atom 19, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.903, -1.625, -1.726
Atom 20, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.903, -1.625, -1.726
Atom 21, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.903, -1.625, -1.726
Atom 22, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.909, -1.625, -1.726
Atom 23, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.903, -1.625, -1.726
Atom 24, -4.191, -3.192, -3.211, -1.770, -1.922, -1.505, -1.498, -1.909, -1.625, -1.726

Ni_9 cluster

Ni1	0.7193335041	1.2459221485	-0.0000000147
Ni2	2.8773339614	-0.0000000080	-0.0000000021
Ni3	2.8773339588	2.4918442978	-0.0000000020
Ni4	-0.6964946252	1.2452165418	2.0447600530
Ni5	3.6195062992	3.7370608401	2.0447600557
Ni6	3.6195063003	-1.2466277535	2.0447600588
Ni7	1.4502816125	-0.0061781655	2.0448054493
Ni8	1.4505954168	2.4967741892	2.0448150202
Ni9	3.6108637762	1.2452202806	2.0147772388

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000090 0.000090 0.000065
vibrational temperatures:

mode:	1	2	3
temp. (K):	20.78	21.14	24.92

Thermodynamic properties calculated assuming an ideal gas

In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 0.066 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	59.995	1.481	-16.406	27.69047
rot.	0.889	2.981	49.194	0.889	-13.778	23.25540
vib.	1.712	5.959	21.447	1.712	-4.683	7.90332
elec.	0.000	0.000	4.366	0.000	-1.302	2.19722
total	3.489	11.920	135.002	4.082	-36.169	61.04641

Total internal energy, Utot (SCFE + ZPE + U): -1523.812006 hartrees
Total enthalpy, Htot (Utot + pV): -1523.811062 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1523.875206 hartrees

Ni_{10} cluster

Ni1	9.3513300000	3.7377600000	2.0345800000
Ni2	9.3513300000	6.2296100000	2.0345800000
Ni3	11.5093300000	4.9836900000	2.0345800000
Ni4	10.0776900000	2.4939200000	4.0405700000
Ni5	7.9172800000	3.7391500000	4.0472900000
Ni6	7.9232000000	6.2291400000	4.0457300000
Ni7	10.0776900000	7.4776000000	4.0405700000
Ni8	12.2374400000	3.7391100000	4.0475200000
Ni9	12.2400500000	6.2308500000	4.0504700000
Ni10	10.0857100000	4.9853000000	4.2392800000

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000080 0.000079 0.000056
vibrational temperatures:

mode:	1	2	3
temp. (K):	20.22	21.92	26.68

Thermodynamic properties calculated assuming an ideal gas

In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 0.068 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.309	1.481	-16.500	27.84851
rot.	0.889	2.981	49.591	0.889	-13.897	23.45526
vib.	1.710	5.959	21.294	1.710	-4.639	7.82958
elec.	0.000	0.000	4.366	0.000	-1.302	2.19722
total	3.487	11.920	135.561	4.080	-36.337	61.33058

Total internal energy, Utot (SCFE + ZPE + U): -1693.106166 hartrees
Total enthalpy, Htot (Utot + pV): -1693.105222 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1693.169631 hartrees

Ni_{12} cluster (used for fcc-top species)

Ni1	1.2459200000	1.4386650000	1.3513016667
Ni2	-1.2459200000	1.4386650000	1.3513016667
Ni3	1.2459200000	-1.4386650000	1.3513016667
Ni4	-1.2459200000	-1.4386650000	1.3513016667
Ni5	2.4918425000	2.1578850000	-0.6755833333
Ni6	2.4918425000	-2.1578850000	-0.6755833333
Ni7	-2.4918425000	2.1578850000	-0.6755833333
Ni8	-2.4918425000	-2.1578850000	-0.6755833333
Ni9	0.0000000000	2.1578850000	-0.6755783333
Ni10	1.2459150000	0.0000000000	-0.6758583333
Ni11	-1.2459150000	0.0000000000	-0.6758583333
Ni12	0.0000000000	-2.1578850000	-0.6755783333

Thermochemical properties at 1.0000 atm
rotational symmetry number: 2
rotational temperatures (K): 0.000054 0.000051 0.000034
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	14.87	19.81	21.42	24.84	27.42	27.75

Thermodynamic properties calculated assuming an ideal gas

In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 0.135 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.852	1.481	-16.662	28.12199
rot.	0.889	2.981	49.514	0.889	-13.874	23.41655
vib.	3.421	11.917	42.903	3.421	-9.370	15.81497
elec.	0.000	0.000	4.765	0.000	-1.421	2.39790
total	5.199	17.879	158.035	5.791	-41.327	69.75140

Total internal energy, Utot (SCFE + ZPE + U): -2031.603814 hartrees
Total enthalpy, Htot (Utot + pV): -2031.602870 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2031.677957 hartrees

Ni_{12} cluster (used for fcc-hcp binding)

Ni1	0.6757983333	-0.5994625000	2.4918400000
Ni2	0.6754683333	3.7167575000	0.0000000000
Ni3	-1.3513116667	2.2777475000	0.0000000000

Ni4	-1.3513116667	0.1197475000	1.2459250000
Ni5	-1.3513116667	0.1197475000	-1.2459250000
Ni6	-1.3513116667	-2.0382525000	0.0000000000
Ni7	0.6757983333	-0.5994625000	-2.4918400000
Ni8	0.6754633333	-2.7572425000	1.2459250000
Ni9	0.6754633333	-2.7572425000	-1.2459250000
Ni10	0.6756783333	1.5585375000	1.2459200000
Ni11	0.6756783333	1.5585375000	-1.2459200000
Ni12	0.6758983333	-0.5994125000	0.0000000000

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000074 0.000044 0.000037
vibrational temperatures:

mode:	1	2	3
temp. (K):	20.10	21.17	24.33

Thermodynamic properties calculated assuming an ideal gas

In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 0.065 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.852	1.481	-16.662	28.12199
rot.	0.889	2.981	50.666	0.889	-14.217	23.99618
vib.	1.713	5.959	21.558	1.713	-4.715	7.95718
elec.	0.000	0.000	3.867	0.000	-1.153	1.94591
total	3.491	11.921	136.944	4.083	-36.747	62.02126

Total internal energy, Utot (SCFE + ZPE + U): -2031.560544 hartrees
Total enthalpy, Htot (Utot + pV): -2031.559600 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2031.624666 hartrees

CH_3CH_3 gas

CH_3CH_3 gas in periodic cell

8 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C	2.12748	1.20199	2.39780
C	2.13088	1.20238	0.85593
H	2.83144	1.93568	2.81188
H	1.13686	1.44549	2.80309
H	2.40745	0.22309	2.80834
H	2.83658	1.93625	0.44557
H	1.14240	1.44622	0.44590
H	2.41304	0.22415	0.44544

FINAL RELAXED ENERGY = -29.9188445682

CH_3CH_3 gas non-periodic calculation

C1	2.1274800000	1.2019900000	2.3978000000
C2	2.1308800000	1.2023800000	0.8559300000
H3	2.8314400000	1.9356800000	2.8118800000
H4	1.1368600000	1.4454900000	2.8030900000
H5	2.4074500000	0.2230900000	2.8083400000
H6	2.8365800000	1.9362500000	0.4455700000
H7	1.1424000000	1.4462200000	0.4459000000
H8	2.4130400000	0.2241500000	0.4454400000

Thermochemical properties at 1.0000 atm

rotational symmetry number: 1
rotational temperatures (K): 3.889004 0.938787 0.938779
1 vibrational frequencies below 10.0 cm-1 not included in zero-point energy or thermochemical analysis. Set freqcut to change the frequency cutoff value.
vibrational temperatures:

mode:	2	3	4	5	6	7
temp. (K):	1300.69	1301.07	1444.33	1693.55	1693.73	2038.73

mode:	8	9	10	11	12	13
temp. (K):	2097.78	2181.96	2182.18	2194.66	2195.10	4392.19

mode:	14	15	16	17	18
temp. (K):	4401.64	4473.06	4473.50	4503.03	4503.60

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature are kelvins, the units for U, H, and G are kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 46.770 kcal/mol is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	36.134	1.481	-9.292	15.68327
rot.	0.889	2.981	19.878	0.889	-5.038	8.50285
vib.	0.132	2.268	0.532	0.132	-0.027	0.04493
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.909	8.230	56.543	2.502	-14.357	24.23105

Total internal energy, Utot (SCFE + ZPE + U): -79.755206 hartrees
Total enthalpy, Htot (Utot + pV): -79.754261 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -79.781127 hartrees

CH_4 gas

CH_4 gas in periodic cell

5 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.24532 1.15017 2.13400
H 2.53005 2.14222 2.50061
H 1.24151 0.90280 2.49678
H 2.96000 0.40462 2.49968
H 2.24600 1.15087 1.03881

FINAL RELAXED ENERGY = -16.1600067313

CH_4 gas in non-periodic calculation

C1	-0.0000324444	0.0000046782	0.0000000000
H2	1.0836053304	-0.0000732163	0.0000000000
H3	-0.3611341470	1.0217004941	0.0000000000
H4	-0.3610424368	-0.5108414904	0.8847956974
H5	-0.3610424368	-0.5108414904	-0.8847956974

Thermochemical properties at 1.0000 atm
rotational symmetry number: 3
rotational temperatures (K): 7.568306 7.568306 7.567146
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	1950.70	1954.32	1954.32	2273.20	2273.20	4395.61

mode:	7	8	9
temp. (K):	4565.83	4565.83	4566.37

Thermodynamic properties calculated assuming an ideal gas

In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 28.317 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	34.261	1.481	-8.734	14.74094
rot.	0.889	2.981	12.886	0.889	-2.953	4.98427
vib.	0.021	0.480	0.081	0.021	-0.003	0.00527
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.799	6.442	47.228	2.391	-11.690	19.73048

Total internal energy, Utot (SCFE + ZPE + U): -40.475240 hartrees
Total enthalpy, Htot (Utot + pV): -40.474295 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -40.496735 hartrees

H_2

H_2 gas in periodic cell

2 4.98369 4.98369 23.01920 90.00000 90.00000 90.00000

H 2.24906 1.24594 5.13305
H 2.24902 1.24595 4.38251

FINAL RELAXED ENERGY = -2.3311760070

H_2 gas non-periodic calculation

H1 0.0000000000 0.0000000000 0.3662957656
H2 0.0000000000 0.0000000000 -0.3662957656

Thermochemical properties at 1.0000 atm
rotational symmetry number: 2
rotational temperatures (K): 87.250383 87.250383
vibrational temperatures:
mode: 1
temp. (K): 6449.74

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 6.408 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	28.080	1.481	-6.891	11.63054
rot.	0.592	1.987	3.052	0.592	-0.317	0.53567
vib.	0.000	0.000	0.000	0.000	0.000	0.00000
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.481	4.968	31.132	2.074	-7.208	12.16620

Total internal energy, Utot (SCFE + ZPE + U): -1.165966 hartrees
Total enthalpy, Htot (Utot + pV): -1.165022 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1.179813 hartrees

Diamond

Diamond in periodic cell

8 3.56683 3.56683 3.56683 90.00000 90.00000 90.00000

C 0.00000 0.00000 0.00000
C 0.00000 1.78342 1.78342
C 1.78342 1.78342 0.00000
C 1.78342 0.00000 1.78342
C 2.67512 0.89171 2.67512

C 0.89171 0.89171 0.89171
C 0.89171 2.67512 2.67512
C 2.67512 2.67512 0.89171

FINAL RELAXED ENERGY = -91.1543049783

CH_2CH_3 binding at top site

$\underline{CH_2CH_3}$ adsorbed in periodic cell

31 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000
Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.44329 0.00139 4.04729
Ni 1.44920 2.49138 4.04573
Ni 3.61171 1.24753 4.23928
Ni 3.60369 3.73984 4.04057
Ni 5.76345 0.00135 4.04752
Ni 5.76605 2.49309 4.05047
C 3.53479 1.23812 6.22885
H 2.74240 1.96267 6.46995
H 3.16195 0.23352 6.47851
C 4.82419 1.55516 6.97016
H 4.64306 1.54297 8.06198
H 5.61797 0.82407 6.75944
H 5.21653 2.55163 6.71626
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2275.4117717883

Total electrons from output= 253
Spin up from output= 134.5000000000
Spin down from output= 118.5000000000
Fermi level up from output= -4.6009653288
Fermi level down from output= -4.6568018904
# of atoms= 31

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.014, -0.013, -0.017, 0.150, 0.140, 0.138, 0.148, 0.169, 0.716
Atom 2, 0.015, -0.014, -0.013, -0.017, 0.148, 0.142, 0.145, 0.151, 0.164, 0.721
Atom 3, 0.013, -0.014, -0.013, -0.016, 0.148, 0.139, 0.136, 0.143, 0.162, 0.700
Atom 4, 0.016, -0.013, -0.014, -0.017, 0.156, 0.150, 0.138, 0.146, 0.162, 0.724
Atom 5, 0.014, -0.014, -0.013, -0.016, 0.147, 0.146, 0.145, 0.147, 0.161, 0.717
Atom 6, 0.014, -0.014, -0.013, -0.017, 0.148, 0.148, 0.146, 0.147, 0.166, 0.727
Atom 7, 0.013, -0.012, -0.012, -0.017, 0.147, 0.144, 0.138, 0.139, 0.171, 0.711
Atom 8, 0.013, -0.013, -0.012, -0.014, 0.138, 0.132, 0.126, 0.141, 0.173, 0.685
Atom 9, 0.015, -0.013, -0.011, -0.017, 0.146, 0.107, 0.138, 0.139, 0.177, 0.683
Atom 10, 0.015, -0.012, -0.011, -0.017, 0.147, 0.106, 0.142, 0.139, 0.178, 0.685
Atom 11, 0.015, -0.012, -0.012, -0.017, 0.146, 0.149, 0.101, 0.145, 0.177, 0.692
Atom 12, 0.014, -0.013, -0.012, -0.016, 0.140, 0.143, 0.138, 0.144, 0.170, 0.708
Atom 13, 0.012, -0.014, -0.016, -0.009, 0.153, 0.113, 0.112, 0.140, 0.178, 0.670
Atom 14, 0.013, -0.014, -0.016, -0.008, 0.151, 0.115, 0.113, 0.140, 0.170, 0.663
Atom 15, 0.005, -0.017, -0.016, -0.008, 0.124, 0.029, 0.030, 0.110, 0.067, 0.323
Atom 16, 0.012, -0.016, -0.013, -0.006, 0.149, 0.128, 0.107, 0.133, 0.157, 0.651
Atom 17, 0.013, -0.014, -0.016, -0.009, 0.153, 0.112, 0.113, 0.137, 0.175, 0.665
Atom 18, 0.013, -0.014, -0.016, -0.008, 0.154, 0.110, 0.105, 0.136, 0.184, 0.664
Atom 19, 0.000, 0.001, -0.000, 0.002, -0.000, -0.000, -0.000, -0.000, -0.000, 0.002
Atom 20, -0.003, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.003
Atom 21, -0.003, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.003
Atom 22, -0.000, -0.000, 0.000, -0.001, -0.000, -0.000, -0.000, 0.000, 0.000, -0.001
Atom 23, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 24, -0.002, -0.000, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 25, -0.002, 0.000, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 26, 0.012, -0.015, -0.015, -0.012, 0.154, 0.115, 0.105, 0.140, 0.203, 0.687
Atom 27, 0.014, -0.015, -0.015, -0.011, 0.153, 0.115, 0.114, 0.139, 0.219, 0.714
Atom 28, 0.009, -0.015, -0.016, -0.014, 0.155, 0.111, 0.107, 0.141, 0.200, 0.677
Atom 29, 0.009, -0.014, -0.015, -0.013, 0.154, 0.110, 0.110, 0.139, 0.197, 0.676
Atom 30, 0.009, -0.015, -0.015, -0.014, 0.154, 0.111, 0.108, 0.140, 0.191, 0.669
Atom 31, 0.012, -0.015, -0.016, -0.012, 0.153, 0.109, 0.101, 0.141, 0.197, 0.671
total spin= 16.1930008066937

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.270, 0.331, 0.332, 0.335, 1.745, 1.768, 1.770, 1.744, 1.709, 10.003
Atom 2, 0.270, 0.330, 0.332, 0.334, 1.748, 1.767, 1.769, 1.741, 1.714, 10.006
Atom 3, 0.269, 0.331, 0.332, 0.336, 1.747, 1.767, 1.771, 1.746, 1.710, 10.008
Atom 4, 0.271, 0.331, 0.332, 0.334, 1.742, 1.767, 1.772, 1.745, 1.715, 10.007
Atom 5, 0.270, 0.330, 0.332, 0.336, 1.747, 1.766, 1.767, 1.744, 1.709, 10.003
Atom 6, 0.270, 0.331, 0.333, 0.336, 1.747, 1.764, 1.767, 1.744, 1.707, 9.998
Atom 7, 0.264, 0.333, 0.332, 0.341, 1.747, 1.771, 1.767, 1.750, 1.706, 10.010
Atom 8, 0.262, 0.330, 0.331, 0.344, 1.754, 1.769, 1.771, 1.748, 1.701, 10.009
Atom 9, 0.281, 0.328, 0.327, 0.321, 1.742, 1.786, 1.768, 1.747, 1.707, 10.007
Atom 10, 0.281, 0.329, 0.327, 0.322, 1.741, 1.786, 1.765, 1.748, 1.707, 10.006
Atom 11, 0.281, 0.325, 0.328, 0.321, 1.746, 1.759, 1.790, 1.737, 1.706, 9.993
Atom 12, 0.264, 0.332, 0.334, 0.342, 1.753, 1.766, 1.768, 1.745, 1.706, 10.011
Atom 13, 0.427, 0.303, 0.299, 0.166, 1.728, 1.807, 1.801, 1.732, 1.736, 9.999
Atom 14, 0.417, 0.303, 0.299, 0.168, 1.731, 1.804, 1.802, 1.732, 1.744, 9.999
Atom 15, 0.382, 0.295, 0.294, 0.279, 1.738, 1.906, 1.901, 1.732, 1.520, 10.047
Atom 16, 0.419, 0.306, 0.297, 0.164, 1.728, 1.788, 1.804, 1.734, 1.754, 9.992
Atom 17, 0.419, 0.299, 0.304, 0.170, 1.728, 1.804, 1.798, 1.734, 1.740, 9.995
Atom 18, 0.416, 0.306, 0.307, 0.170, 1.726, 1.805, 1.807, 1.734, 1.730, 10.001
Atom 19, 1.306, 0.990, 1.067, 1.010, 0.009, 0.004, 0.007, 0.005, 0.005, 4.404

Atom 20, 0.809, 0.006, 0.005, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.824
Atom 21, 0.810, 0.003, 0.008, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.824
Atom 22, 1.275, 0.995, 1.099, 1.036, 0.009, 0.002, 0.005, 0.005, 0.011, 4.435
Atom 23, 0.831, 0.003, 0.003, 0.008, 0.000, 0.000, 0.000, 0.000, 0.000, 0.845
Atom 24, 0.820, 0.006, 0.005, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.834
Atom 25, 0.820, 0.003, 0.008, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.834
Atom 26, 0.441, 0.300, 0.299, 0.166, 1.728, 1.803, 1.810, 1.732, 1.712, 9.989
Atom 27, 0.441, 0.300, 0.300, 0.166, 1.729, 1.804, 1.802, 1.733, 1.700, 9.975
Atom 28, 0.439, 0.300, 0.299, 0.164, 1.728, 1.807, 1.809, 1.732, 1.716, 9.993
Atom 29, 0.439, 0.300, 0.299, 0.164, 1.727, 1.805, 1.806, 1.733, 1.714, 9.987
Atom 30, 0.439, 0.299, 0.300, 0.164, 1.728, 1.806, 1.805, 1.732, 1.719, 9.992
Atom 31, 0.441, 0.299, 0.299, 0.165, 1.729, 1.805, 1.811, 1.731, 1.718, 9.999

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.154, -3.919, -3.901, -4.073, -2.066, -1.812, -1.794, -2.057, -2.193, -2.184
Atom 2, -5.154, -3.919, -3.892, -4.073, -2.075, -1.830, -1.848, -2.057, -2.211, -2.193
Atom 3, -5.163, -3.901, -3.892, -4.064, -2.066, -1.803, -1.794, -2.048, -2.184, -2.175
Atom 4, -5.172, -3.901, -3.892, -4.082, -2.075, -1.857, -1.839, -2.066, -2.202, -2.193
Atom 5, -5.163, -3.910, -3.892, -4.064, -2.066, -1.812, -1.812, -2.048, -2.184, -2.184
Atom 6, -5.163, -3.919, -3.892, -4.064, -2.066, -1.821, -1.821, -2.057, -2.193, -2.184
Atom 7, -5.209, -3.883, -3.919, -4.073, -2.057, -1.821, -1.866, -2.048, -2.202, -2.202
Atom 8, -5.191, -3.955, -3.937, -4.046, -2.039, -1.839, -1.839, -2.012, -2.211, -2.202
Atom 9, -5.127, -3.892, -3.883, -4.073, -2.030, -1.657, -1.739, -2.012, -2.148, -2.121
Atom 10, -5.136, -3.883, -3.874, -4.064, -2.030, -1.667, -1.748, -2.003, -2.148, -2.130
Atom 11, -5.136, -3.837, -3.828, -4.073, -2.012, -1.757, -1.639, -2.030, -2.139, -2.121
Atom 12, -5.236, -3.919, -3.855, -4.082, -2.075, -1.839, -1.848, -2.057, -2.211, -2.202
Atom 13, -4.264, -3.174, -3.192, -2.157, -1.912, -1.494, -1.476, -1.884, -1.567, -1.721
Atom 14, -4.328, -3.229, -3.211, -2.330, -1.894, -1.494, -1.485, -1.875, -1.576, -1.712
Atom 15, -4.373, -3.383, -3.465, -2.393, -1.803, -1.240, -1.285, -1.830, -2.693, -1.821
Atom 16, -4.337, -3.092, -3.283, -2.357, -1.894, -1.512, -1.512, -1.848, -1.567, -1.721
Atom 17, -4.319, -3.192, -3.147, -2.266, -1.894, -1.494, -1.503, -1.884, -1.594, -1.712
Atom 18, -4.328, -3.201, -3.165, -2.502, -1.903, -1.503, -1.494, -1.894, -1.594, -1.730
Atom 19, -14.100, -4.945, -5.000, -2.675, -4.128, -1.594, -4.437, -4.636, -2.784, -5.972
Atom 20, -6.280, -6.598, -6.716, -3.002, -14.509, -14.509, -14.509, -14.509, -14.509, -6.280
Atom 21, -6.280, -6.299, -5.027, -3.056, -14.509, -14.509, -14.509, -14.509, -14.509, -6.280
Atom 22, -14.164, -4.900, -4.882, -5.835, -4.128, -6.417, -5.163, -4.782, -2.511, -5.990
Atom 23, -5.863, -4.909, -4.864, -10.467, -14.509, -14.509, -14.509, -14.509, -14.509, -5.863
Atom 24, -5.018, -6.517, -6.580, -5.808, -14.509, -14.509, -14.509, -14.509, -14.509, -5.036
Atom 25, -5.054, -5.300, -4.991, -5.808, -14.509, -14.509, -14.509, -14.509, -14.509, -5.091
Atom 26, -4.164, -3.183, -3.192, -1.785, -1.903, -1.485, -1.485, -1.884, -1.603, -1.712
Atom 27, -4.164, -3.183, -3.192, -1.766, -1.903, -1.494, -1.494, -1.884, -1.612, -1.712
Atom 28, -4.182, -3.183, -3.192, -1.794, -1.894, -1.485, -1.485, -1.884, -1.576, -1.703
Atom 29, -4.173, -3.183, -3.201, -1.785, -1.894, -1.485, -1.476, -1.875, -1.594, -1.694
Atom 30, -4.182, -3.192, -3.183, -1.803, -1.894, -1.485, -1.476, -1.875, -1.576, -1.703
Atom 31, -4.164, -3.192, -3.192, -1.775, -1.894, -1.485, -1.476, -1.884, -1.585, -1.703

CH_2CH_3 adsorbed on Ni_{10} cluster

Ni1	9.3513300000	3.7377599998	2.0345800001
Ni2	9.3513299999	6.2296100000	2.0345800000
Ni3	11.5093300000	4.9836900000	2.0345800000
Ni4	10.0776900000	2.4939200000	4.0405700000
Ni5	7.9172800000	3.7391500000	4.0472900000
Ni6	7.9232000000	6.2291400000	4.0457300000
Ni7	10.0776900000	7.4776000000	4.0405700000

Ni8	12.2374400000	3.7391100000	4.0475200000
Ni9	12.2400500000	6.2308500000	4.0504700000
Ni10	10.0857100001	4.9853000004	4.2392799999
C11	10.0947437483	5.0587407400	6.2268885802
H12	9.5151243559	5.9520666282	6.4912589370
H13	9.4926416751	4.1933051112	6.5275919642
C14	11.4252299422	5.0612472107	6.9827243418
H15	11.2700894988	5.1279388833	8.0708548149
H16	12.0080302389	4.1497446054	6.7956378763
H17	12.0626932877	5.9107608642	6.6980185271

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000079 0.000079 0.000056
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	20.46	22.36	26.64	124.57	147.49	336.32
mode:	7	8	9	10	11	12
temp. (K):	354.88	442.03	652.92	1105.32	1434.21	1439.60
mode:	13	14	15	16	17	18
temp. (K):	1506.98	1773.27	1863.12	2035.34	2143.42	2156.84
mode:	19	20	21	22	23	24
temp. (K):	2163.01	4305.68	4391.98	4420.57	4461.53	4567.67

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 41.628 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.310	1.481	-16.500	27.84895
rot.	0.889	2.981	49.593	0.889	-13.898	23.45635
vib.	3.845	18.888	34.759	3.845	-6.518	11.00093
elec.	0.000	0.000	4.132	0.000	-1.232	2.07944
total	5.623	24.849	148.794	6.215	-38.148	64.38567

Total internal energy, Utot (SCFE + ZPE + U): -1772.244933 hartrees
Total enthalpy, Htot (Utot + pV): -1772.243989 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1772.314686 hartrees

C_2CH_3 gas

CH_2CH_3 gas in periodic cell

7 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.13186 1.19336 2.41713
C 2.15879 1.19439 0.93248
H 2.82234 1.94275 2.84404

H 1.13262 1.45348 2.81169
H 2.40517 0.21640 2.83583
H 1.93709 2.10498 0.37704
H 2.38313 0.29460 0.36357

FINAL RELAXED ENERGY = -28.5977685874

CH_2CH_3 gas in non-periodic calculation

C1	9.9767567668	4.9683030696	6.3516920602
H2	9.2300219685	5.7410502065	6.2018870743
H3	9.6617259671	3.9373801686	6.2288380651
C4	11.3150499797	5.2973660082	6.9158667404
H5	11.3059536523	5.3192447041	8.0199628414
H6	12.0718437695	4.5586602526	6.6281524987
H7	11.6630299731	6.2847330905	6.5911006945

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 4.964450 1.087861 1.008516
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 171.09 669.49 1171.53 1417.22 1541.51 1724.77
mode: 7 8 9 10 11 12
temp. (K): 2033.06 2128.76 2151.51 2153.05 4264.68 4397.45
mode: 13 14 15
temp. (K): 4463.93 4549.19 4695.45

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 37.293 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	36.032	1.481	-9.262	15.63209
rot.	0.889	2.981	19.418	0.889	-4.901	8.27126
vib.	0.710	5.127	4.330	0.710	-0.581	0.98121
elec.	0.000	0.000	1.377	0.000	-0.411	0.69315
total	2.487	11.089	61.157	3.079	-15.154	25.57771

Total internal energy, Utot (SCFE + ZPE + U): -79.100205 hartrees
Total enthalpy, Htot (Utot + pV): -79.099260 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -79.128318 hartrees

$CHCH_3$ binding at fcc site

$CHCH_3$ adsorbed in periodic cell

30 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000
Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.45876 -0.00617 4.12434
Ni 1.46427 2.49645 4.12262
Ni 3.63884 1.24844 4.10547
Ni 3.63530 3.73437 4.04681
Ni 5.75846 -0.00414 4.03794
Ni 5.79077 2.49183 4.04544
C 2.10519 1.24170 5.46605
H 3.23497 1.20330 5.77693
C 1.40048 1.27407 6.81056
H 0.31427 1.37036 6.69261
H 1.76151 2.12068 7.41699
H 1.60375 0.34902 7.37516
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2274.2232616217

Total electrons from output= 252
Spin up from output= 134.0000000000
Spin down from output= 118.0000000000
Fermi level up from output= -4.3415647724
Fermi level down from output= -4.425700566
# of atoms= 30

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.014, -0.015, 0.157, 0.146, 0.140, 0.148, 0.165, 0.728
Atom 2, 0.016, -0.014, -0.014, -0.016, 0.156, 0.148, 0.127, 0.150, 0.161, 0.713
Atom 3, 0.016, -0.014, -0.014, -0.016, 0.152, 0.167, 0.153, 0.148, 0.165, 0.757
Atom 4, 0.014, -0.014, -0.013, -0.014, 0.155, 0.155, 0.144, 0.149, 0.158, 0.734
Atom 5, 0.015, -0.014, -0.015, -0.017, 0.153, 0.146, 0.156, 0.151, 0.167, 0.742
Atom 6, 0.015, -0.014, -0.015, -0.018, 0.154, 0.145, 0.157, 0.151, 0.172, 0.747
Atom 7, 0.015, -0.013, -0.009, -0.013, 0.154, 0.093, 0.140, 0.149, 0.197, 0.714
Atom 8, 0.016, -0.011, -0.009, -0.014, 0.151, 0.074, 0.117, 0.148, 0.167, 0.638
Atom 9, 0.015, -0.011, -0.011, -0.014, 0.150, 0.137, 0.121, 0.148, 0.196, 0.730
Atom 10, 0.015, -0.012, -0.011, -0.014, 0.150, 0.138, 0.126, 0.146, 0.197, 0.736
Atom 11, 0.012, -0.012, -0.012, -0.013, 0.145, 0.142, 0.129, 0.147, 0.162, 0.700
Atom 12, 0.013, -0.012, -0.013, -0.015, 0.142, 0.137, 0.137, 0.147, 0.172, 0.708
Atom 13, 0.002, -0.014, -0.007, -0.008, 0.097, 0.058, 0.061, 0.113, 0.053, 0.354

Atom 14, 0.001, -0.014, -0.007, -0.009, 0.097, 0.059, 0.062, 0.113, 0.054, 0.356
Atom 15, 0.006, -0.012, -0.014, -0.010, 0.131, 0.053, 0.061, 0.112, 0.181, 0.507
Atom 16, 0.017, -0.009, -0.009, -0.003, 0.180, 0.109, 0.125, 0.147, 0.184, 0.741
Atom 17, 0.019, -0.013, -0.012, -0.008, 0.152, 0.133, 0.113, 0.165, 0.177, 0.725
Atom 18, 0.019, -0.013, -0.014, -0.008, 0.168, 0.118, 0.139, 0.158, 0.170, 0.738
Atom 19, 0.007, 0.020, -0.002, 0.011, -0.000, 0.000, 0.000, -0.000, -0.000, 0.036
Atom 20, 0.001, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.001
Atom 21, 0.000, 0.001, -0.001, 0.002, 0.000, -0.000, 0.000, 0.000, 0.000, 0.003
Atom 22, 0.002, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.002
Atom 23, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.000
Atom 24, -0.001, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.001
Atom 25, 0.013, -0.015, -0.015, -0.012, 0.161, 0.113, 0.113, 0.144, 0.209, 0.711
Atom 26, 0.013, -0.014, -0.015, -0.011, 0.159, 0.114, 0.118, 0.142, 0.213, 0.718
Atom 27, 0.012, -0.015, -0.016, -0.012, 0.159, 0.119, 0.111, 0.144, 0.202, 0.703
Atom 28, 0.012, -0.014, -0.016, -0.012, 0.161, 0.116, 0.111, 0.144, 0.202, 0.704
Atom 29, 0.017, -0.015, -0.018, -0.008, 0.162, 0.124, 0.119, 0.143, 0.229, 0.753
Atom 30, 0.011, -0.013, -0.015, -0.011, 0.159, 0.122, 0.113, 0.144, 0.215, 0.723
total spin= 16.4211418542772

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.331, 0.331, 0.335, 1.741, 1.770, 1.769, 1.744, 1.712, 10.005
Atom 2, 0.269, 0.331, 0.331, 0.334, 1.742, 1.769, 1.778, 1.742, 1.715, 10.011
Atom 3, 0.270, 0.330, 0.331, 0.335, 1.747, 1.757, 1.764, 1.746, 1.712, 9.992
Atom 4, 0.270, 0.331, 0.332, 0.338, 1.744, 1.757, 1.768, 1.743, 1.714, 9.998
Atom 5, 0.271, 0.332, 0.330, 0.336, 1.746, 1.765, 1.759, 1.741, 1.712, 9.992
Atom 6, 0.271, 0.332, 0.330, 0.336, 1.745, 1.771, 1.757, 1.740, 1.709, 9.991
Atom 7, 0.282, 0.327, 0.330, 0.330, 1.739, 1.791, 1.776, 1.751, 1.693, 10.019
Atom 8, 0.269, 0.327, 0.322, 0.322, 1.739, 1.812, 1.781, 1.744, 1.699, 10.015
Atom 9, 0.283, 0.330, 0.327, 0.331, 1.745, 1.775, 1.786, 1.744, 1.693, 10.013
Atom 10, 0.282, 0.330, 0.328, 0.332, 1.745, 1.774, 1.780, 1.746, 1.693, 10.010
Atom 11, 0.266, 0.333, 0.330, 0.343, 1.749, 1.767, 1.765, 1.745, 1.703, 10.001
Atom 12, 0.261, 0.333, 0.332, 0.344, 1.752, 1.770, 1.764, 1.748, 1.703, 10.007
Atom 13, 0.333, 0.289, 0.299, 0.213, 1.759, 1.719, 1.799, 1.736, 1.767, 9.915
Atom 14, 0.333, 0.291, 0.301, 0.211, 1.762, 1.718, 1.795, 1.736, 1.771, 9.918
Atom 15, 0.336, 0.311, 0.346, 0.246, 1.737, 1.851, 1.787, 1.762, 1.685, 10.060
Atom 16, 0.421, 0.307, 0.281, 0.163, 1.712, 1.821, 1.790, 1.737, 1.735, 9.966
Atom 17, 0.414, 0.294, 0.305, 0.167, 1.723, 1.789, 1.814, 1.730, 1.741, 9.977
Atom 18, 0.430, 0.310, 0.295, 0.175, 1.715, 1.802, 1.774, 1.727, 1.741, 9.969
Atom 19, 1.347, 0.981, 0.993, 1.068, 0.003, 0.006, 0.009, 0.008, 0.011, 4.425
Atom 20, 0.777, 0.009, 0.004, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.796
Atom 21, 1.265, 1.089, 1.079, 0.940, 0.002, 0.009, 0.005, 0.008, 0.006, 4.402
Atom 22, 0.817, 0.009, 0.003, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.831
Atom 23, 0.822, 0.003, 0.006, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.836
Atom 24, 0.820, 0.003, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.834
Atom 25, 0.441, 0.299, 0.300, 0.166, 1.727, 1.805, 1.807, 1.732, 1.709, 9.985
Atom 26, 0.441, 0.299, 0.300, 0.166, 1.727, 1.805, 1.801, 1.732, 1.705, 9.976
Atom 27, 0.441, 0.299, 0.299, 0.166, 1.727, 1.799, 1.805, 1.731, 1.710, 9.977
Atom 28, 0.441, 0.299, 0.299, 0.166, 1.726, 1.803, 1.805, 1.731, 1.712, 9.981
Atom 29, 0.443, 0.301, 0.297, 0.168, 1.728, 1.794, 1.799, 1.731, 1.694, 9.955
Atom 30, 0.440, 0.302, 0.299, 0.166, 1.728, 1.797, 1.804, 1.730, 1.702, 9.967

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.193, -3.921, -3.921, -4.107, -2.093, -1.861, -1.842, -2.084, -2.213, -2.204
Atom 2, -5.221, -3.903, -3.912, -4.079, -2.084, -1.861, -1.824, -2.084, -2.204, -2.195

Atom 3, -5.165, -3.940, -3.921, -3.958, -2.084, -1.851, -1.842, -2.074, -2.223, -2.213
Atom 4, -5.184, -3.912, -3.893, -4.060, -2.102, -1.879, -1.842, -2.074, -2.241, -2.213
Atom 5, -5.184, -3.931, -3.940, -4.107, -2.093, -1.833, -1.870, -2.084, -2.232, -2.223
Atom 6, -5.184, -3.921, -3.931, -4.079, -2.093, -1.851, -1.861, -2.084, -2.232, -2.213
Atom 7, -5.202, -3.921, -3.893, -3.986, -2.046, -1.712, -1.787, -2.009, -2.176, -2.158
Atom 8, -5.137, -3.912, -3.949, -3.996, -1.944, -1.508, -1.657, -1.963, -2.148, -2.093
Atom 9, -5.202, -3.866, -3.819, -4.005, -2.056, -1.731, -1.749, -2.037, -2.186, -2.167
Atom 10, -5.202, -3.884, -3.838, -4.014, -2.065, -1.731, -1.777, -2.037, -2.186, -2.176
Atom 11, -5.193, -3.903, -3.968, -4.005, -2.056, -1.777, -1.814, -2.046, -2.223, -2.204
Atom 12, -5.713, -3.958, -4.005, -4.098, -2.084, -1.824, -1.870, -2.056, -2.223, -2.213
Atom 13, -4.376, -3.169, -3.207, -2.473, -1.963, -1.824, -1.536, -1.981, -1.916, -1.935
Atom 14, -4.395, -3.160, -3.225, -2.538, -1.954, -1.824, -1.536, -1.981, -1.898, -1.935
Atom 15, -5.128, -3.773, -3.207, -4.831, -2.046, -1.684, -1.796, -2.028, -2.269, -2.074
Atom 16, -4.404, -3.132, -3.457, -2.381, -1.889, -1.304, -1.490, -1.842, -1.582, -1.694
Atom 17, -4.376, -3.234, -3.067, -2.353, -1.972, -1.545, -1.415, -1.870, -1.610, -1.749
Atom 18, -4.218, -2.631, -2.900, -1.889, -2.019, -1.471, -1.545, -1.972, -1.592, -1.777
Atom 19, -14.818, -7.198, -5.880, -6.075, -2.111, -3.680, -2.288, -4.525, -4.766, -6.650
Atom 20, -7.235, -11.170, -11.170, -6.121, -15.226, -15.226, -15.226, -15.226, -15.226, -7.235
Atom 21, -14.873, -5.805, -6.223, -6.474, -6.270, -2.947, -6.279, -4.896, -6.000, -6.464
Atom 22, -5.796, -11.142, -11.235, -6.307, -15.226, -15.226, -15.226, -15.226, -15.226, -5.815
Atom 23, -6.307, -6.195, -6.232, -6.334, -15.226, -15.226, -15.226, -15.226, -15.226, -6.307
Atom 24, -6.297, -5.963, -6.112, -6.325, -15.226, -15.226, -15.226, -15.226, -15.226, -6.297
Atom 25, -4.190, -3.207, -3.188, -1.796, -1.916, -1.499, -1.490, -1.898, -1.619, -1.722
Atom 26, -4.181, -3.207, -3.188, -1.796, -1.916, -1.499, -1.499, -1.898, -1.619, -1.731
Atom 27, -4.181, -3.207, -3.207, -1.787, -1.916, -1.499, -1.490, -1.898, -1.610, -1.722
Atom 28, -4.190, -3.207, -3.216, -1.787, -1.916, -1.490, -1.480, -1.898, -1.610, -1.722
Atom 29, -4.181, -3.188, -3.244, -1.768, -1.926, -1.508, -1.508, -1.916, -1.647, -1.749
Atom 30, -4.228, -3.179, -3.216, -1.787, -1.916, -1.499, -1.499, -1.907, -1.629, -1.731

$CHCH_3$ adsorbed on Ni_9 cluster

Ni1	7.1933299910	4.9836899969	2.0345799845
Ni2	9.3513300071	3.7377600055	2.0345799832
Ni3	9.3513300018	6.2296100030	2.0345799911
Ni4	10.1092999983	2.4884500034	4.0468100161
Ni5	5.7584600048	4.9795499998	4.0379400136
Ni6	10.1092999954	7.4721399966	4.0468100156
Ni7	7.9327600841	3.7316001877	4.1243400084
Ni8	7.9382700855	6.2342198193	4.1226199927
Ni9	10.1128398321	4.9862099879	4.1054699948
C10	8.4977138873	4.9749931722	5.6430365227
H11	9.5385524012	4.9471841319	6.0439597891
C12	7.6229815966	4.9875844059	6.8812525790
H13	6.5516257147	5.0150095043	6.6505654148
H14	7.8485363032	5.8622345525	7.5115209417
H15	7.8057677698	4.0999513213	7.5066030261

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000090 0.000089 0.000065
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	16.26	20.90	23.62	117.89	148.08	244.27
mode:	7	8	9	10	11	12
temp. (K):	276.88	339.40	482.68	1006.54	1358.12	1388.46
mode:	13	14	15	16	17	18

temp. (K): 1491.61 1928.83 1987.86 2129.32 2140.51 4057.93
mode: 19 20 21
temp. (K): 4292.49 4357.41 4413.38

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 32.016 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	59.996	1.481	-16.406	27.69094
rot.	0.889	2.981	49.216	0.889	-13.785	23.26655
vib.	4.119	19.418	37.695	4.119	-7.120	12.01745
elec.	0.000	0.000	3.198	0.000	-0.954	1.60944
total	5.896	25.380	150.105	6.489	-38.265	64.58438

Total internal energy, Utot (SCFE + ZPE + U): -1602.325042 hartrees
Total enthalpy, Htot (Utot + pV): -1602.324097 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1602.395417 hartrees

$CHCH_3$ gas

<u>$CHCH_3$ gas in periodic cell</u>

6 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.10319 1.30607 2.52906
C 2.03970 1.14468 1.07812
H 2.08858 2.37109 2.82831
H 3.01249 0.85570 2.97180
H 1.24130 0.82584 3.02007
H 2.57624 1.57590 0.23708

FINAL RELAXED ENERGY = -27.2491369298

<u>$CHCH_3$ gas in non-periodic calculation</u>

C1	8.5953510727	4.7978704706	5.5491922541
H2	9.6591934540	5.0621283133	5.7550347999
C3	7.8682376519	5.1253703318	6.7757608598
H4	6.7774560675	5.1596997400	6.6849476668
H5	8.2407215803	5.8775243075	7.4880716553
H6	8.0955638509	4.1265538750	7.2350434760

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 5.837139 1.270479 1.193711
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 699.87 880.41 1382.37 1612.44 1834.43 1895.42

mode: 7 8 9 10 11 12
temp. (K): 1969.33 2200.49 4110.85 4171.83 4327.86 4457.99

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 29.354 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.927	1.481	-9.230	15.57911
rot.	0.889	2.981	18.935	0.889	-4.757	8.02841
vib.	0.307	3.458	1.376	0.307	-0.103	0.17418
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	2.085	9.420	56.238	2.677	-14.090	23.78169

Total internal energy, Utot (SCFE + ZPE + U): -78.419204 hartrees
Total enthalpy, Htot (Utot + pV): -78.418260 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -78.444980 hartrees

CCH_3 binding at fcc site

CCH_3 adsorbed in periodic cell

29 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni	0.00000	0.00000	0.00000
Ni	0.00000	2.49184	0.00000
Ni	2.15800	1.24592	0.00000
Ni	2.15800	3.73776	0.00000
Ni	4.31600	0.00000	0.00000
Ni	4.31600	2.49184	0.00000
Ni	0.71933	1.24592	2.03458
Ni	0.71933	3.73776	2.03458
Ni	2.87733	0.00000	2.03458
Ni	2.87733	2.49184	2.03458
Ni	5.03533	1.24592	2.03458
Ni	5.03533	3.73776	2.03458
Ni	1.43197	-0.00462	4.12802
Ni	1.43315	2.50074	4.12691
Ni	3.60353	1.24975	4.13377
Ni	3.61849	3.73785	4.06279
Ni	5.73085	0.00396	4.06036
Ni	5.76170	2.49068	4.05141
C	2.15237	1.24879	5.31318
C	2.14398	1.25570	6.80445
H	3.17145	1.26225	7.19754
H	1.62844	0.36492	7.19349
H	1.62137	2.14590	7.18543
Ni	1.43867	0.00000	-2.03458
Ni	1.43867	2.49184	-2.03458

Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2273.0621524198

Total electrons from output= 251
Spin up from output= 133.0000000000
Spin down from output= 118.0000000000
Fermi level up from output= -4.3751292942
Fermi level down from output= -4.4312923854
# of atoms= 29

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.015, -0.013, -0.015, -0.016, 0.153, 0.141, 0.139, 0.144, 0.162, 0.711
Atom 2, 0.016, -0.014, -0.015, -0.016, 0.154, 0.143, 0.140, 0.147, 0.156, 0.712
Atom 3, 0.015, -0.013, -0.014, -0.015, 0.149, 0.159, 0.146, 0.144, 0.164, 0.734
Atom 4, 0.015, -0.013, -0.014, -0.014, 0.153, 0.163, 0.148, 0.144, 0.154, 0.736
Atom 5, 0.014, -0.013, -0.016, -0.015, 0.148, 0.141, 0.147, 0.146, 0.156, 0.709
Atom 6, 0.014, -0.013, -0.015, -0.017, 0.149, 0.143, 0.153, 0.146, 0.164, 0.724
Atom 7, 0.015, -0.012, -0.010, -0.011, 0.153, 0.091, 0.129, 0.142, 0.197, 0.694
Atom 8, 0.016, -0.011, -0.010, -0.012, 0.147, 0.069, 0.107, 0.141, 0.159, 0.606
Atom 9, 0.014, -0.011, -0.011, -0.012, 0.144, 0.125, 0.104, 0.141, 0.194, 0.689
Atom 10, 0.014, -0.011, -0.011, -0.012, 0.145, 0.129, 0.112, 0.143, 0.194, 0.703
Atom 11, 0.014, -0.012, -0.013, -0.015, 0.144, 0.143, 0.081, 0.142, 0.167, 0.652
Atom 12, 0.013, -0.013, -0.012, -0.016, 0.138, 0.136, 0.136, 0.144, 0.170, 0.696
Atom 13, -0.002, -0.009, -0.009, -0.008, 0.072, 0.045, 0.047, 0.064, 0.029, 0.229
Atom 14, -0.003, -0.010, -0.008, -0.009, 0.076, 0.047, 0.049, 0.064, 0.029, 0.234
Atom 15, -0.003, -0.010, -0.013, -0.009, 0.086, 0.054, 0.046, 0.074, 0.037, 0.262
Atom 16, 0.019, -0.009, -0.007, -0.001, 0.163, 0.111, 0.119, 0.120, 0.175, 0.690
Atom 17, 0.017, -0.008, -0.010, -0.004, 0.130, 0.128, 0.105, 0.154, 0.165, 0.677
Atom 18, 0.016, -0.012, -0.011, -0.006, 0.135, 0.114, 0.123, 0.137, 0.147, 0.644
Atom 19, 0.005, -0.017, -0.012, 0.006, -0.000, 0.000, 0.000, -0.000, -0.000, -0.018
Atom 20, 0.001, 0.000, 0.000, 0.003, -0.000, -0.000, -0.000, -0.000, 0.000, 0.004
Atom 21, -0.002, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 22, -0.002, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 23, -0.002, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 24, 0.014, -0.016, -0.014, -0.010, 0.158, 0.113, 0.110, 0.140, 0.210, 0.707
Atom 25, 0.017, -0.015, -0.014, -0.009, 0.157, 0.113, 0.124, 0.140, 0.220, 0.733
Atom 26, 0.012, -0.014, -0.017, -0.013, 0.156, 0.118, 0.111, 0.141, 0.195, 0.690
Atom 27, 0.010, -0.013, -0.016, -0.013, 0.158, 0.115, 0.113, 0.141, 0.197, 0.692
Atom 28, 0.014, -0.015, -0.018, -0.011, 0.158, 0.122, 0.118, 0.141, 0.214, 0.723
Atom 29, 0.010, -0.014, -0.016, -0.012, 0.155, 0.118, 0.115, 0.141, 0.207, 0.704
total spin= 15.3324416961799

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.270, 0.332, 0.331, 0.334, 1.743, 1.775, 1.773, 1.744, 1.715, 10.016
Atom 2, 0.271, 0.331, 0.331, 0.333, 1.744, 1.772, 1.773, 1.742, 1.722, 10.017
Atom 3, 0.269, 0.331, 0.331, 0.335, 1.749, 1.761, 1.767, 1.745, 1.715, 10.003
Atom 4, 0.271, 0.331, 0.332, 0.338, 1.746, 1.755, 1.764, 1.744, 1.719, 10.001
Atom 5, 0.270, 0.332, 0.329, 0.337, 1.748, 1.768, 1.763, 1.741, 1.716, 10.005
Atom 6, 0.270, 0.332, 0.330, 0.336, 1.747, 1.771, 1.760, 1.740, 1.712, 9.998
Atom 7, 0.283, 0.325, 0.329, 0.328, 1.739, 1.799, 1.785, 1.748, 1.688, 10.023

Atom 8, 0.269, 0.326, 0.321, 0.322, 1.740, 1.817, 1.788, 1.742, 1.701, 10.026
Atom 9, 0.284, 0.327, 0.327, 0.327, 1.745, 1.787, 1.794, 1.744, 1.688, 10.023
Atom 10, 0.284, 0.328, 0.327, 0.328, 1.743, 1.784, 1.787, 1.744, 1.688, 10.012
Atom 11, 0.269, 0.324, 0.330, 0.329, 1.745, 1.759, 1.814, 1.744, 1.697, 10.011
Atom 12, 0.267, 0.330, 0.333, 0.339, 1.754, 1.769, 1.772, 1.745, 1.705, 10.013
Atom 13, 0.336, 0.310, 0.309, 0.218, 1.767, 1.697, 1.782, 1.740, 1.807, 9.965
Atom 14, 0.334, 0.311, 0.309, 0.218, 1.769, 1.697, 1.782, 1.738, 1.807, 9.966
Atom 15, 0.328, 0.299, 0.317, 0.214, 1.739, 1.824, 1.662, 1.766, 1.806, 9.956
Atom 16, 0.420, 0.292, 0.285, 0.169, 1.716, 1.802, 1.797, 1.747, 1.738, 9.967
Atom 17, 0.429, 0.291, 0.297, 0.175, 1.731, 1.787, 1.804, 1.726, 1.745, 9.986
Atom 18, 0.434, 0.309, 0.296, 0.185, 1.716, 1.796, 1.772, 1.730, 1.760, 9.998
Atom 19, 1.411, 0.893, 0.896, 1.006, 0.004, 0.008, 0.008, 0.004, 0.014, 4.245
Atom 20, 1.282, 1.088, 1.089, 0.951, 0.004, 0.006, 0.007, 0.004, 0.008, 4.438
Atom 21, 0.816, 0.008, 0.003, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.830
Atom 22, 0.815, 0.004, 0.007, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.829
Atom 23, 0.815, 0.004, 0.007, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.829
Atom 24, 0.442, 0.299, 0.300, 0.168, 1.728, 1.804, 1.808, 1.733, 1.710, 9.991
Atom 25, 0.443, 0.299, 0.300, 0.168, 1.728, 1.805, 1.793, 1.733, 1.700, 9.969
Atom 26, 0.441, 0.300, 0.299, 0.166, 1.728, 1.801, 1.805, 1.730, 1.719, 9.989
Atom 27, 0.440, 0.300, 0.299, 0.166, 1.727, 1.802, 1.803, 1.730, 1.715, 9.982
Atom 28, 0.441, 0.301, 0.297, 0.167, 1.729, 1.795, 1.802, 1.730, 1.704, 9.965
Atom 29, 0.440, 0.301, 0.298, 0.166, 1.730, 1.799, 1.803, 1.729, 1.707, 9.971

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.163, -3.886, -3.895, -4.096, -2.079, -1.851, -1.842, -2.070, -2.198, -2.180
Atom 2, -5.218, -3.877, -3.886, -4.078, -2.079, -1.869, -1.860, -2.079, -2.207, -2.189
Atom 3, -5.118, -3.895, -3.895, -3.941, -2.070, -1.851, -1.842, -2.052, -2.198, -2.189
Atom 4, -5.127, -3.895, -3.886, -4.078, -2.088, -1.897, -1.860, -2.061, -2.216, -2.198
Atom 5, -5.182, -3.904, -3.922, -4.087, -2.070, -1.833, -1.851, -2.061, -2.207, -2.189
Atom 6, -5.172, -3.904, -3.913, -4.068, -2.070, -1.851, -1.851, -2.061, -2.207, -2.189
Atom 7, -5.145, -3.895, -3.877, -3.968, -2.015, -1.669, -1.696, -1.979, -2.143, -2.125
Atom 8, -5.099, -3.932, -3.950, -4.014, -1.906, -1.450, -1.596, -1.933, -2.107, -2.052
Atom 9, -5.136, -3.849, -3.822, -3.959, -1.997, -1.687, -1.669, -1.997, -2.143, -2.116
Atom 10, -5.163, -3.831, -3.804, -3.959, -2.006, -1.687, -1.687, -2.006, -2.143, -2.125
Atom 11, -5.136, -3.932, -3.895, -4.059, -1.997, -1.732, -1.550, -1.979, -2.152, -2.125
Atom 12, -5.273, -3.904, -3.904, -4.059, -2.052, -1.805, -1.805, -2.043, -2.207, -2.180
Atom 13, -4.406, -3.338, -3.293, -2.645, -1.970, -1.970, -1.586, -2.024, -1.851, -1.997
Atom 14, -4.433, -3.375, -3.320, -2.654, -1.970, -1.988, -1.586, -2.043, -1.860, -1.997
Atom 15, -4.488, -3.402, -3.256, -2.700, -2.034, -1.477, -2.243, -2.024, -1.851, -2.006
Atom 16, -4.388, -3.065, -3.183, -2.143, -1.787, -1.331, -1.459, -1.751, -1.568, -1.669
Atom 17, -4.269, -3.092, -3.028, -1.805, -1.906, -1.523, -1.395, -1.851, -1.568, -1.705
Atom 18, -4.105, -2.581, -2.818, -1.687, -1.997, -1.486, -1.541, -1.924, -1.532, -1.751
Atom 19, -10.510, -3.649, -3.612, -6.213, -1.815, -3.886, -3.859, -1.805, -2.216, -6.423
Atom 20, -14.708, -6.459, -6.432, -6.359, -6.350, -3.056, -3.092, -6.413, -6.879, -6.514
Atom 21, -6.477, -10.410, -10.520, -6.459, -15.036, -15.036, -15.036, -15.036, -15.036, -6.477
Atom 22, -6.441, -6.477, -6.468, -6.423, -15.036, -15.036, -15.036, -15.036, -15.036, -6.441
Atom 23, -6.432, -6.486, -6.468, -6.423, -15.036, -15.036, -15.036, -15.036, -15.036, -6.432
Atom 24, -4.169, -3.192, -3.174, -1.751, -1.897, -1.486, -1.477, -1.888, -1.605, -1.705
Atom 25, -4.178, -3.192, -3.174, -1.751, -1.906, -1.495, -1.486, -1.888, -1.614, -1.723
Atom 26, -4.187, -3.192, -3.211, -1.778, -1.906, -1.486, -1.468, -1.888, -1.596, -1.705
Atom 27, -4.187, -3.183, -3.211, -1.778, -1.897, -1.477, -1.459, -1.888, -1.596, -1.705
Atom 28, -4.178, -3.183, -3.229, -1.769, -1.906, -1.486, -1.486, -1.897, -1.614, -1.723
Atom 29, -4.242, -3.183, -3.229, -1.778, -1.897, -1.477, -1.477, -1.888, -1.605, -1.714

CCH_3 adsorbed on Ni_9 cluster

Ni1	7.1933299981	4.9836900009	2.0345799979
Ni2	9.3513300002	3.7377600022	2.0345799967
Ni3	9.3513299995	6.2296100006	2.0345799983
Ni4	10.0924899998	2.4919300005	4.0627900018
Ni5	5.7308500008	4.9876499996	4.0603600024
Ni6	10.0924900000	7.4756099991	4.0627900024
Ni7	7.9059700211	3.7331400421	4.1280200032
Ni8	7.9071400267	6.2384999535	4.1269099944
Ni9	10.0775299538	4.9875200015	4.1337700028
C10	8.6199856059	4.9979432514	5.2628401458
C11	8.5932671730	5.0297216227	6.7595395051
H12	9.6124739219	5.0416266335	7.1691790588
H13	8.0774582276	4.1468874509	7.1611276134
H14	8.0709860317	5.9215370272	7.1309639254

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000089 0.000088 0.000065
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	15.92	21.06	21.53	43.56	168.95	175.65
mode:	7	8	9	10	11	12
temp. (K):	516.82	644.10	661.27	1394.40	1396.69	1575.49
mode:	13	14	15	16	17	18
temp. (K):	1973.52	2094.46	2097.88	4319.51	4422.68	4425.00

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 25.802 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	59.996	1.481	-16.406	27.69092
rot.	0.889	2.981	49.228	0.889	-13.789	23.27242
vib.	3.774	17.469	37.315	3.774	-7.352	12.40806
elec.	0.000	0.000	2.755	0.000	-0.821	1.38629
total	5.551	23.430	149.293	6.144	-38.368	64.75771

Total internal energy, Utot (SCFE + ZPE + U): -1601.732226 hartrees
Total enthalpy, Htot (Utot + pV): -1601.731282 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1601.802216 hartrees

CCH_3 gas

CCH_3 gas in periodic cell

5 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.03937 1.11206 1.71211
C 2.00712 0.98298 0.27108
H 2.68874 2.02578 1.69266
H 2.59104 0.34415 2.28930
H 1.10112 1.40245 2.22308

FINAL RELAXED ENERGY = -25.9347885821

CCH_3 gas in non-periodic calculation

C1	8.5745770064	5.0743143651	5.3412455075
C2	8.6664250842	4.9110588610	6.7816891232
H3	9.6660847969	4.9971296238	7.2379111114
H4	8.0997251759	4.0793080625	7.2322437509
H5	8.1173130116	5.8462914355	7.0431438088

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 7.650931 1.383174 1.371319
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 775.03 1220.32 1570.43 1900.35 1907.73 2103.16
mode: 7 8 9
temp. (K): 4182.74 4300.05 4341.06

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 22.158 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.818	1.481	-9.198	15.52418
rot.	0.889	2.981	18.444	0.889	-4.610	7.78127
vib.	0.197	2.387	0.868	0.197	-0.061	0.10346
elec.	0.000	0.000	1.377	0.000	-0.411	0.69315
total	1.975	8.348	56.507	2.567	-14.280	24.10206

Total internal energy, Utot (SCFE + ZPE + U): -77.789079 hartrees
Total enthalpy, Htot (Utot + pV): -77.788135 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -77.814983 hartrees

CH_2CH_2 binding at fcc-top site

CH_2CH_3 adsorbed in periodic cell

30 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000

Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.41940 -0.00078 4.08101
Ni 1.42096 2.49325 4.08181
Ni 3.59906 1.24861 4.18914
Ni 3.60287 3.73675 4.00881
Ni 5.72632 0.00076 4.03722
Ni 5.74824 2.49153 4.04813
C 2.13955 1.25347 5.83954
C 3.54065 1.26258 6.17987
H 1.56677 0.33701 6.09747
H 1.55531 2.16484 6.09319
H 3.98470 0.34785 6.57665
H 3.97621 2.18537 6.56770
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2274.2360014442

Total electrons from output= 252
Spin up from output= 134.5000000000
Spin down from output= 117.5000000000
Fermi level up from output= -4.236925641
Fermi level down from output= -4.3847755228
# of atoms= 30

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.012, -0.011, -0.015, 0.161, 0.146, 0.145, 0.160, 0.173, 0.763
Atom 2, 0.016, -0.013, -0.011, -0.015, 0.157, 0.144, 0.143, 0.163, 0.171, 0.756
Atom 3, 0.016, -0.013, -0.012, -0.017, 0.156, 0.150, 0.147, 0.158, 0.168, 0.753
Atom 4, 0.019, -0.013, -0.013, -0.017, 0.161, 0.158, 0.149, 0.160, 0.173, 0.778
Atom 5, 0.017, -0.013, -0.012, -0.017, 0.157, 0.154, 0.162, 0.161, 0.172, 0.782
Atom 6, 0.017, -0.013, -0.012, -0.017, 0.157, 0.154, 0.163, 0.161, 0.175, 0.785
Atom 7, 0.017, -0.011, -0.010, -0.016, 0.161, 0.154, 0.142, 0.156, 0.188, 0.782
Atom 8, 0.014, -0.011, -0.010, -0.010, 0.147, 0.122, 0.142, 0.158, 0.172, 0.724
Atom 9, 0.016, -0.011, -0.009, -0.012, 0.155, 0.120, 0.139, 0.156, 0.187, 0.742
Atom 10, 0.016, -0.010, -0.008, -0.012, 0.155, 0.119, 0.144, 0.155, 0.187, 0.744
Atom 11, 0.016, -0.010, -0.010, -0.014, 0.154, 0.160, 0.119, 0.159, 0.188, 0.761
Atom 12, 0.015, -0.011, -0.011, -0.014, 0.147, 0.146, 0.152, 0.157, 0.180, 0.760
Atom 13, 0.013, -0.015, -0.013, -0.008, 0.149, 0.085, 0.089, 0.148, 0.177, 0.625
Atom 14, 0.012, -0.015, -0.013, -0.007, 0.143, 0.086, 0.088, 0.148, 0.177, 0.618
Atom 15, -0.000, -0.009, -0.018, -0.006, 0.123, 0.027, 0.039, 0.115, 0.091, 0.362
Atom 16, 0.018, -0.013, -0.015, -0.008, 0.174, 0.149, 0.124, 0.158, 0.164, 0.751
Atom 17, 0.018, -0.013, -0.014, -0.005, 0.171, 0.129, 0.122, 0.156, 0.176, 0.741

Atom 18, 0.021, -0.011, -0.014, -0.006, 0.173, 0.127, 0.125, 0.159, 0.188, 0.761
Atom 19, 0.002, -0.001, 0.007, 0.006, -0.000, 0.000, -0.000, -0.000, -0.000, 0.014
Atom 20, 0.000, 0.001, 0.000, -0.003, 0.000, -0.000, -0.000, -0.000, 0.000, -0.001
Atom 21, -0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.005
Atom 22, -0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.005
Atom 23, -0.002, 0.000, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 24, -0.002, 0.000, -0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 25, 0.013, -0.013, -0.014, -0.011, 0.165, 0.119, 0.111, 0.151, 0.217, 0.740
Atom 26, 0.017, -0.013, -0.015, -0.010, 0.165, 0.120, 0.122, 0.149, 0.229, 0.765
Atom 27, 0.014, -0.013, -0.015, -0.009, 0.166, 0.115, 0.113, 0.150, 0.215, 0.736
Atom 28, 0.017, -0.012, -0.016, -0.006, 0.167, 0.110, 0.116, 0.149, 0.221, 0.747
Atom 29, 0.011, -0.013, -0.015, -0.014, 0.166, 0.117, 0.122, 0.150, 0.208, 0.732
Atom 30, 0.015, -0.013, -0.016, -0.011, 0.166, 0.118, 0.116, 0.153, 0.220, 0.748
total spin= 17.4535621043552

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.333, 0.334, 0.338, 1.742, 1.767, 1.767, 1.748, 1.707, 10.006
Atom 2, 0.270, 0.332, 0.334, 0.337, 1.745, 1.767, 1.767, 1.746, 1.710, 10.008
Atom 3, 0.270, 0.332, 0.334, 0.334, 1.747, 1.762, 1.769, 1.749, 1.711, 10.007
Atom 4, 0.273, 0.332, 0.332, 0.334, 1.742, 1.758, 1.768, 1.747, 1.714, 10.001
Atom 5, 0.273, 0.332, 0.334, 0.337, 1.746, 1.759, 1.759, 1.747, 1.711, 9.999
Atom 6, 0.272, 0.333, 0.334, 0.336, 1.747, 1.759, 1.759, 1.746, 1.709, 9.995
Atom 7, 0.275, 0.332, 0.336, 0.339, 1.742, 1.766, 1.777, 1.752, 1.703, 10.023
Atom 8, 0.269, 0.329, 0.332, 0.347, 1.752, 1.765, 1.770, 1.749, 1.705, 10.017
Atom 9, 0.279, 0.327, 0.331, 0.332, 1.745, 1.774, 1.775, 1.747, 1.703, 10.013
Atom 10, 0.279, 0.328, 0.331, 0.332, 1.744, 1.775, 1.772, 1.747, 1.703, 10.012
Atom 11, 0.277, 0.330, 0.334, 0.333, 1.748, 1.758, 1.783, 1.745, 1.693, 10.000
Atom 12, 0.259, 0.333, 0.338, 0.349, 1.755, 1.759, 1.763, 1.752, 1.705, 10.013
Atom 13, 0.360, 0.314, 0.319, 0.201, 1.736, 1.806, 1.825, 1.728, 1.728, 10.017
Atom 14, 0.358, 0.313, 0.320, 0.203, 1.741, 1.804, 1.827, 1.729, 1.732, 10.026
Atom 15, 0.336, 0.321, 0.327, 0.296, 1.762, 1.916, 1.816, 1.743, 1.593, 10.110
Atom 16, 0.402, 0.311, 0.292, 0.164, 1.721, 1.785, 1.798, 1.730, 1.757, 9.959
Atom 17, 0.418, 0.295, 0.308, 0.168, 1.712, 1.789, 1.810, 1.733, 1.744, 9.978
Atom 18, 0.427, 0.310, 0.304, 0.173, 1.711, 1.795, 1.808, 1.727, 1.731, 9.986
Atom 19, 1.296, 0.958, 1.082, 1.010, 0.012, 0.003, 0.008, 0.007, 0.005, 4.380
Atom 20, 1.263, 0.920, 1.069, 0.957, 0.008, 0.006, 0.007, 0.008, 0.004, 4.241
Atom 21, 0.775, 0.004, 0.007, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.791
Atom 22, 0.773, 0.004, 0.007, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.789
Atom 23, 0.814, 0.004, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.829
Atom 24, 0.815, 0.004, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.830
Atom 25, 0.442, 0.302, 0.301, 0.166, 1.727, 1.800, 1.809, 1.734, 1.703, 9.984
Atom 26, 0.443, 0.302, 0.300, 0.166, 1.729, 1.800, 1.799, 1.735, 1.693, 9.968
Atom 27, 0.442, 0.302, 0.300, 0.168, 1.728, 1.807, 1.806, 1.733, 1.704, 9.991
Atom 28, 0.445, 0.302, 0.299, 0.170, 1.727, 1.807, 1.802, 1.734, 1.702, 9.988
Atom 29, 0.440, 0.302, 0.301, 0.164, 1.727, 1.803, 1.802, 1.735, 1.709, 9.982
Atom 30, 0.442, 0.301, 0.300, 0.165, 1.728, 1.801, 1.809, 1.733, 1.704, 9.984

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.196, -3.945, -3.906, -4.100, -2.120, -1.848, -1.839, -2.110, -2.256, -2.246
Atom 2, -5.206, -3.935, -3.896, -4.080, -2.110, -1.868, -1.878, -2.101, -2.237, -2.237
Atom 3, -5.187, -3.935, -3.915, -3.993, -2.110, -1.839, -1.839, -2.101, -2.246, -2.237
Atom 4, -5.158, -3.935, -3.935, -4.119, -2.130, -1.897, -1.868, -2.110, -2.266, -2.256
Atom 5, -5.177, -3.945, -3.906, -4.109, -2.120, -1.868, -1.878, -2.101, -2.256, -2.256
Atom 6, -5.148, -3.945, -3.906, -4.129, -2.120, -1.868, -1.878, -2.110, -2.256, -2.256

Atom 7, -5.187, -3.886, -3.847, -4.032, -2.130, -1.907, -1.848, -2.091, -2.256, -2.246
Atom 8, -5.187, -3.945, -3.867, -3.974, -2.081, -1.878, -1.839, -2.062, -2.285, -2.237
Atom 9, -5.216, -3.915, -3.838, -3.974, -2.081, -1.751, -1.771, -2.072, -2.198, -2.188
Atom 10, -5.216, -3.915, -3.847, -3.974, -2.081, -1.751, -1.781, -2.072, -2.198, -2.188
Atom 11, -5.206, -3.877, -3.867, -4.051, -2.072, -1.868, -1.781, -2.091, -2.285, -2.237
Atom 12, -5.487, -4.032, -3.974, -4.158, -2.110, -1.946, -1.936, -2.101, -2.285, -2.266
Atom 13, -4.973, -3.013, -3.149, -4.546, -1.946, -1.586, -1.596, -1.975, -1.771, -1.858
Atom 14, -4.983, -3.013, -3.120, -4.546, -1.916, -1.596, -1.586, -1.946, -1.771, -1.848
Atom 15, -5.662, -3.750, -3.401, -4.012, -2.004, -1.557, -1.790, -1.994, -2.964, -2.110
Atom 16, -4.323, -3.226, -3.488, -2.402, -1.946, -1.528, -1.596, -1.916, -1.616, -1.790
Atom 17, -4.304, -3.265, -3.003, -2.324, -2.033, -1.567, -1.431, -1.936, -1.635, -1.781
Atom 18, -4.274, -2.935, -3.052, -2.237, -2.033, -1.528, -1.460, -2.023, -1.625, -1.800
Atom 19, -15.453, -7.098, -7.137, -4.866, -5.439, -1.781, -2.392, -7.108, -3.246, -8.001
Atom 20, -15.395, -6.953, -5.662, -3.605, -5.449, -2.062, -3.877, -7.079, -4.323, -7.098
Atom 21, -8.001, -8.059, -7.147, -5.158, -15.803, -15.803, -15.803, -15.803, -15.803, -8.001
Atom 22, -8.001, -8.059, -7.157, -5.138, -15.803, -15.803, -15.803, -15.803, -15.803, -8.001
Atom 23, -7.069, -5.701, -7.059, -5.128, -15.803, -15.803, -15.803, -15.803, -15.803, -7.069
Atom 24, -7.069, -5.662, -7.050, -5.022, -15.803, -15.803, -15.803, -15.803, -15.803, -7.069
Atom 25, -4.226, -3.188, -3.207, -1.839, -1.955, -1.538, -1.528, -1.936, -1.664, -1.761
Atom 26, -4.226, -3.197, -3.217, -1.829, -1.955, -1.538, -1.538, -1.936, -1.674, -1.771
Atom 27, -4.226, -3.197, -3.217, -1.810, -1.946, -1.528, -1.528, -1.926, -1.645, -1.761
Atom 28, -4.207, -3.197, -3.236, -1.790, -1.955, -1.519, -1.519, -1.936, -1.654, -1.761
Atom 29, -4.216, -3.197, -3.207, -1.858, -1.955, -1.528, -1.528, -1.936, -1.654, -1.761
Atom 30, -4.236, -3.197, -3.217, -1.839, -1.955, -1.528, -1.528, -1.936, -1.654, -1.761

CH_2CH_3 adsorbed on Ni_{12} cluster

Ni1	10.0773999949	2.4912899965	4.0081200119
Ni2	5.7285100080	4.9845699816	4.0363400025
Ni3	7.1933299847	4.9836900116	2.0345799974
Ni4	9.3513300050	3.7377599908	2.0345799957
Ni5	9.3513299984	6.2296099981	2.0345799999
Ni6	11.5093300000	4.9836900052	2.0345800000
Ni7	10.0773999964	7.4749800069	4.0081200050
Ni8	12.2025100013	3.7386500022	4.0363400004
Ni9	12.2239200014	6.2302399976	4.0472600004
Ni10	7.8956299759	3.7376500407	4.0822899939
Ni11	7.8963800471	6.2315199488	4.0826799962
Ni12	10.0762899869	4.9869100199	4.1867999967
C13	8.0946036090	5.0442526379	5.9898235501
C14	9.5285103385	4.9743655266	6.1723225103
H15	7.5140239853	4.1823067625	6.3375084768
H16	7.6114120793	5.9882251409	6.2794727962
H17	9.9515180668	4.0477706763	6.5520944209
H18	10.0484768316	5.8681887236	6.5118310378

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000074 0.000044 0.000037
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	23.09	24.29	28.05	285.10	296.91	492.11
mode:	7	8	9	10	11	12
temp. (K):	560.29	768.95	1306.63	1471.93	1592.96	1610.93
mode:	13	14	15	16	17	18
temp. (K):	1652.64	1712.77	1892.25	2162.19	2235.62	4501.98

mode: 19 20 21
temp. (K): 4646.54 4653.36 4803.52

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 36.487 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.853	1.481	-16.662	28.12234
rot.	0.889	2.981	50.674	0.889	-14.220	23.99988
vib.	3.081	15.998	28.215	3.081	-5.331	8.99843
elec.	0.000	0.000	3.867	0.000	-1.153	1.94591
total	4.858	21.960	143.609	5.451	-37.366	63.06656

Total internal energy, Utot (SCFE + ZPE + U): -2110.308717 hartrees
Total enthalpy, Htot (Utot + pV): -2110.307773 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2110.376006 hartrees

CH_2CH_2 gas

CH_2CH_2 gas in periodic cell

6 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.14739 1.18324 2.24984
C 2.23958 1.25327 0.92236
H 1.79679 2.07852 0.36349
H 2.76353 0.49109 0.34398
H 2.59069 0.35961 2.81142
H 1.62593 1.94760 2.82719

FINAL RELAXED ENERGY = -27.4627365215

CH_2CH_2 gas in non-periodic calculation

C1	8.6568277260	4.9903058029	5.9194355138
C2	9.9609172576	4.9987609268	6.1841370042
H3	8.0998512624	4.0634904309	5.8092240016
H4	8.0894436078	5.9100387063	5.8025075073
H5	10.5279772812	4.0788710403	6.3005841203
H6	10.5173039664	5.9258171468	6.2945029268

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 7.056185 1.442861 1.197910
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 1195.43 1384.13 1406.17 1537.55 1783.75 1994.68
mode: 7 8 9 10 11 12

temp. (K): 2132.47 2466.16 4525.27 4547.26 4633.89 4670.99

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 32.071 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.927	1.481	-9.230	15.57911
rot.	0.889	2.981	18.617	0.889	-4.662	7.86820
vib.	0.132	2.139	0.537	0.132	-0.028	0.04756
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.910	8.100	55.081	2.502	-13.920	23.49487

Total internal energy, Utot (SCFE + ZPE + U): -78.537799 hartrees
Total enthalpy, Htot (Utot + pV): -78.536854 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -78.563025 hartrees

CCH_2 binding at fcc-top site

CCH_2 adsorbed in periodic cell

28 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000
Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.42979 -0.01636 4.11847
Ni 1.42828 2.50469 4.12025
Ni 3.67853 1.24626 4.15114
Ni 3.62018 3.73514 4.02848
Ni 5.75622 -0.00922 4.05560
Ni 5.77779 2.49548 4.04766
C 2.13346 1.24441 5.30085
C 3.11633 1.22833 6.27556
H 3.39591 0.29612 6.77274
H 3.42519 2.14656 6.78075
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458

Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2271.8385988667

Total electrons from output= 250
Spin up from output= 133.0000000000
Spin down from output= 117.0000000000
Fermi level up from output= -4.551210381
Fermi level down from output= -4.653591016
# of atoms= 28

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.016, -0.013, -0.013, -0.015, 0.158, 0.148, 0.141, 0.149, 0.166, 0.736
Atom 2, 0.016, -0.014, -0.013, -0.016, 0.157, 0.151, 0.129, 0.152, 0.161, 0.724
Atom 3, 0.015, -0.014, -0.013, -0.016, 0.152, 0.160, 0.152, 0.149, 0.162, 0.748
Atom 4, 0.016, -0.013, -0.013, -0.015, 0.158, 0.164, 0.140, 0.151, 0.159, 0.745
Atom 5, 0.015, -0.013, -0.015, -0.017, 0.154, 0.145, 0.154, 0.153, 0.164, 0.739
Atom 6, 0.015, -0.013, -0.014, -0.018, 0.155, 0.145, 0.158, 0.153, 0.172, 0.752
Atom 7, 0.016, -0.013, -0.009, -0.014, 0.156, 0.097, 0.141, 0.150, 0.206, 0.733
Atom 8, 0.015, -0.012, -0.008, -0.013, 0.151, 0.064, 0.116, 0.146, 0.161, 0.621
Atom 9, 0.015, -0.011, -0.010, -0.014, 0.150, 0.133, 0.122, 0.148, 0.193, 0.726
Atom 10, 0.015, -0.011, -0.010, -0.015, 0.151, 0.133, 0.128, 0.146, 0.194, 0.732
Atom 11, 0.013, -0.011, -0.011, -0.013, 0.144, 0.150, 0.113, 0.148, 0.159, 0.691
Atom 12, 0.013, -0.012, -0.011, -0.013, 0.142, 0.137, 0.137, 0.148, 0.174, 0.713
Atom 13, 0.001, -0.014, -0.007, -0.009, 0.084, 0.071, 0.058, 0.097, 0.050, 0.331
Atom 14, 0.000, -0.014, -0.007, -0.009, 0.083, 0.071, 0.057, 0.097, 0.048, 0.327
Atom 15, -0.001, -0.011, -0.014, -0.007, 0.117, 0.040, 0.047, 0.091, 0.157, 0.419
Atom 16, 0.018, -0.008, -0.010, -0.004, 0.172, 0.130, 0.126, 0.141, 0.176, 0.742
Atom 17, 0.017, -0.012, -0.011, -0.007, 0.149, 0.134, 0.127, 0.160, 0.179, 0.736
Atom 18, 0.019, -0.013, -0.013, -0.008, 0.168, 0.128, 0.146, 0.150, 0.162, 0.739
Atom 19, 0.010, 0.014, -0.016, -0.000, -0.000, -0.000, 0.000, -0.000, -0.000, 0.008
Atom 20, 0.004, 0.008, 0.001, 0.015, -0.000, -0.000, 0.000, -0.000, -0.000, 0.028
Atom 21, -0.004, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.003
Atom 22, -0.003, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.003
Atom 23, 0.013, -0.016, -0.013, -0.013, 0.163, 0.111, 0.113, 0.146, 0.212, 0.717
Atom 24, 0.016, -0.015, -0.014, -0.012, 0.159, 0.112, 0.123, 0.144, 0.222, 0.737
Atom 25, 0.012, -0.014, -0.016, -0.015, 0.160, 0.117, 0.113, 0.145, 0.200, 0.702
Atom 26, 0.011, -0.014, -0.015, -0.014, 0.162, 0.112, 0.116, 0.146, 0.200, 0.704
Atom 27, 0.015, -0.014, -0.017, -0.011, 0.161, 0.125, 0.120, 0.145, 0.222, 0.748
Atom 28, 0.011, -0.012, -0.015, -0.012, 0.159, 0.121, 0.113, 0.146, 0.217, 0.728
total spin= 16.317332086652

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.332, 0.332, 0.335, 1.741, 1.769, 1.771, 1.746, 1.713, 10.010
Atom 2, 0.270, 0.330, 0.332, 0.333, 1.742, 1.768, 1.781, 1.743, 1.717, 10.015
Atom 3, 0.269, 0.330, 0.332, 0.335, 1.748, 1.762, 1.766, 1.746, 1.712, 10.000
Atom 4, 0.271, 0.331, 0.333, 0.337, 1.743, 1.753, 1.771, 1.743, 1.716, 9.997
Atom 5, 0.271, 0.332, 0.331, 0.337, 1.746, 1.768, 1.761, 1.742, 1.712, 9.999
Atom 6, 0.271, 0.332, 0.331, 0.337, 1.744, 1.770, 1.756, 1.741, 1.710, 9.993
Atom 7, 0.281, 0.328, 0.330, 0.326, 1.739, 1.795, 1.771, 1.750, 1.689, 10.010
Atom 8, 0.264, 0.327, 0.325, 0.327, 1.739, 1.812, 1.778, 1.744, 1.702, 10.018
Atom 9, 0.286, 0.330, 0.326, 0.326, 1.743, 1.778, 1.782, 1.746, 1.696, 10.013
Atom 10, 0.286, 0.329, 0.326, 0.326, 1.742, 1.777, 1.778, 1.747, 1.696, 10.006

Atom 11, 0.269, 0.331, 0.330, 0.333, 1.749, 1.759, 1.777, 1.744, 1.706, 9.997
Atom 12, 0.264, 0.333, 0.335, 0.346, 1.753, 1.764, 1.768, 1.749, 1.704, 10.014
Atom 13, 0.334, 0.300, 0.320, 0.236, 1.754, 1.704, 1.790, 1.753, 1.785, 9.977
Atom 14, 0.336, 0.301, 0.320, 0.235, 1.756, 1.702, 1.790, 1.752, 1.783, 9.977
Atom 15, 0.359, 0.307, 0.335, 0.282, 1.728, 1.879, 1.795, 1.759, 1.656, 10.100
Atom 16, 0.407, 0.306, 0.282, 0.161, 1.714, 1.801, 1.793, 1.745, 1.745, 9.953
Atom 17, 0.407, 0.286, 0.301, 0.161, 1.725, 1.790, 1.801, 1.730, 1.737, 9.937
Atom 18, 0.417, 0.313, 0.298, 0.172, 1.714, 1.799, 1.766, 1.732, 1.748, 9.959
Atom 19, 1.381, 0.882, 0.922, 0.914, 0.006, 0.007, 0.010, 0.009, 0.011, 4.143
Atom 20, 1.266, 0.979, 1.056, 0.917, 0.004, 0.010, 0.005, 0.006, 0.005, 4.249
Atom 21, 0.804, 0.003, 0.008, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.819
Atom 22, 0.804, 0.004, 0.007, 0.004, 0.000, 0.000, 0.000, 0.000, 0.000, 0.819
Atom 23, 0.441, 0.299, 0.301, 0.165, 1.726, 1.806, 1.807, 1.733, 1.708, 9.985
Atom 24, 0.442, 0.300, 0.301, 0.165, 1.727, 1.806, 1.796, 1.733, 1.699, 9.968
Atom 25, 0.441, 0.300, 0.300, 0.164, 1.727, 1.801, 1.804, 1.731, 1.712, 9.980
Atom 26, 0.440, 0.300, 0.300, 0.165, 1.726, 1.803, 1.802, 1.731, 1.714, 9.981
Atom 27, 0.442, 0.302, 0.298, 0.166, 1.728, 1.793, 1.797, 1.731, 1.700, 9.957
Atom 28, 0.440, 0.302, 0.299, 0.166, 1.728, 1.796, 1.803, 1.730, 1.703, 9.967

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.153, -3.922, -3.912, -4.118, -2.103, -1.869, -1.841, -2.093, -2.233, -2.215
Atom 2, -5.200, -3.912, -3.903, -4.099, -2.093, -1.879, -1.841, -2.093, -2.224, -2.205
Atom 3, -5.191, -3.940, -3.922, -3.959, -2.093, -1.841, -1.860, -2.075, -2.224, -2.215
Atom 4, -5.181, -3.912, -3.903, -4.062, -2.112, -1.907, -1.869, -2.084, -2.252, -2.233
Atom 5, -5.200, -3.931, -3.931, -4.118, -2.103, -1.832, -1.879, -2.093, -2.243, -2.224
Atom 6, -5.228, -3.922, -3.931, -4.080, -2.112, -1.860, -1.879, -2.084, -2.243, -2.224
Atom 7, -5.209, -3.875, -3.894, -3.968, -2.047, -1.720, -1.785, -2.028, -2.187, -2.177
Atom 8, -5.209, -3.978, -3.968, -3.987, -1.953, -1.496, -1.646, -1.953, -2.140, -2.084
Atom 9, -5.144, -3.838, -3.819, -3.978, -2.056, -1.720, -1.739, -2.047, -2.177, -2.168
Atom 10, -5.191, -3.856, -3.829, -3.978, -2.056, -1.711, -1.748, -2.047, -2.177, -2.168
Atom 11, -5.200, -3.838, -3.903, -3.922, -2.037, -1.757, -1.739, -2.028, -2.205, -2.177
Atom 12, -5.209, -3.959, -3.968, -4.099, -2.084, -1.851, -1.879, -2.065, -2.243, -2.224
Atom 13, -4.398, -3.213, -3.315, -2.616, -2.056, -1.907, -1.636, -2.028, -1.944, -2.028
Atom 14, -4.454, -3.185, -3.325, -2.625, -2.056, -1.897, -1.627, -2.037, -1.953, -2.028
Atom 15, -5.293, -3.735, -3.371, -3.437, -2.075, -1.590, -1.925, -2.112, -2.476, -2.131
Atom 16, -4.388, -3.138, -3.474, -2.327, -1.860, -1.384, -1.524, -1.795, -1.608, -1.720
Atom 17, -4.351, -3.371, -3.101, -2.327, -2.000, -1.562, -1.412, -1.879, -1.627, -1.767
Atom 18, -4.220, -2.709, -3.064, -2.075, -2.075, -1.534, -1.590, -1.972, -1.608, -1.823
Atom 19, -14.883, -5.181, -4.621, -6.012, -2.849, -3.241, -4.351, -2.746, -2.271, -6.431
Atom 20, -14.939, -4.640, -6.581, -6.151, -2.886, -2.933, -14.930, -6.469, -4.845, -6.860
Atom 21, -6.907, -4.323, -6.422, -6.823, -15.294, -15.294, -15.294, -15.294, -15.294, -6.907
Atom 22, -6.916, -4.416, -6.450, -6.823, -15.294, -15.294, -15.294, -15.294, -15.294, -6.916
Atom 23, -4.220, -3.222, -3.185, -1.823, -1.925, -1.506, -1.506, -1.907, -1.636, -1.739
Atom 24, -4.220, -3.203, -3.185, -1.813, -1.925, -1.515, -1.515, -1.907, -1.636, -1.748
Atom 25, -4.220, -3.203, -3.213, -1.832, -1.925, -1.506, -1.506, -1.907, -1.618, -1.729
Atom 26, -4.202, -3.213, -3.213, -1.804, -1.925, -1.496, -1.487, -1.907, -1.618, -1.739
Atom 27, -4.183, -3.194, -3.241, -1.795, -1.935, -1.515, -1.515, -1.925, -1.646, -1.757
Atom 28, -4.239, -3.185, -3.222, -1.804, -1.925, -1.506, -1.506, -1.916, -1.636, -1.748

CCH_2 adsorbed on Ni_{12} cluster

Ni1	10.0941800031	2.4892200093	4.0284799959
Ni2	5.7562200018	4.9744700000	4.0556000047
Ni3	7.1933300123	4.9836900069	2.0345799869
Ni4	9.3513299943	3.7377600002	2.0345799998

Ni5	9.3513299929	6.2296099923	2.0345799994
Ni6	11.5093300004	4.9836900117	2.0345800002
Ni7	10.0941800020	7.4728999954	4.0284799937
Ni8	12.2302200088	3.7285500137	4.0556000109
Ni9	12.2517900093	6.2332399852	4.0476600109
Ni10	7.9037900180	3.7214001172	4.1184700224
Ni11	7.9022800311	6.2424598767	4.1202500082
Ni12	10.1525299259	4.9840199913	4.1511399669
C13	8.5085581444	4.9890252842	5.3846659310
C14	9.3926505801	4.9644917713	6.4195362891
H15	9.7013958407	4.0332502492	6.8986442117
H16	9.7039525835	5.8765646551	6.9337496087

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000074 0.000043 0.000036
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	23.24	25.78	29.59	326.05	348.73	602.16
mode:	7	8	9	10	11	12
temp. (K):	771.20	821.94	1296.78	1401.78	1547.07	2036.77
mode:	13	14	15			
temp. (K):	2269.63	4540.91	4675.86			

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 20.585 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.853	1.481	-16.662	28.12232
rot.	0.889	2.981	50.692	0.889	-14.225	24.00893
vib.	2.841	14.591	26.491	2.841	-5.058	8.53607
elec.	0.000	0.000	3.198	0.000	-0.954	1.60944
total	4.618	20.553	141.233	5.211	-36.898	62.27676

Total internal energy, Utot (SCFE + ZPE + U): -2109.105242 hartrees
Total enthalpy, Htot (Utot + pV): -2109.104298 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2109.171402 hartrees

CCH_2 gas

CCH_2 gas in periodic cell

4 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 1.90061 0.25377 1.20671
C 2.16779 1.47643 1.53447
H 1.87958 2.47554 1.18923

H 2.88853 1.42304 2.37235

FINAL RELAXED ENERGY = -24.8298657126

CCH_2 gas in non-periodic calculation

C1	8.6713151830	4.9818234138	5.3022324926
C2	9.5255629283	4.9664479078	6.2860284212
H3	9.8754506447	4.0220141304	6.7025286951
H4	9.9045070579	5.8961801339	6.7098545046

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 13.699592 1.880290 1.653364
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	528.43	1087.49	1768.25	2472.79	4522.41	4635.25

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 14.919 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.704	1.481	-9.164	15.46717
rot.	0.889	2.981	17.374	0.889	-4.291	7.24296
vib.	0.283	2.487	1.379	0.283	-0.128	0.21556
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	2.061	8.448	54.457	2.653	-13.583	22.92569

Total internal energy, Utot (SCFE + ZPE + U): -77.233934 hartrees
Total enthalpy, Htot (Utot + pV): -77.232990 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -77.258864 hartrees

$CHCH_2$ binding at fcc-top site

$CHCH_2$ adsorbed in periodic cell

29 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni	0.00000	0.00000	0.00000
Ni	0.00000	2.49184	0.00000
Ni	2.15800	1.24592	0.00000
Ni	2.15800	3.73776	0.00000
Ni	4.31600	0.00000	0.00000
Ni	4.31600	2.49184	0.00000
Ni	0.71933	1.24592	2.03458
Ni	0.71933	3.73776	2.03458
Ni	2.87733	0.00000	2.03458
Ni	2.87733	2.49184	2.03458

Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.42074 0.00447 4.13196
Ni 1.43197 2.51787 4.07480
Ni 3.64742 1.26873 4.15460
Ni 3.61851 3.74284 4.01256
Ni 5.74414 0.00203 4.04132
Ni 5.76693 2.50504 4.04859
C 2.11615 1.17030 5.48928
C 3.32393 0.93206 6.18973
H 3.67695 -0.08457 6.37521
H 3.71241 1.68316 6.88523
H 1.54398 2.08025 5.87833
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2273.0179023127

Total electrons from output= 251
Spin up from output= 133.5000000000
Spin down from output= 117.5000000000
Fermi level up from output= -4.4532378956
Fermi level down from output= -4.5305709892
# of atoms= 29

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.014, -0.012, -0.012, -0.015, 0.155, 0.131, 0.137, 0.148, 0.165, 0.710
Atom 2, 0.017, -0.014, -0.013, -0.017, 0.157, 0.154, 0.128, 0.154, 0.165, 0.731
Atom 3, 0.014, -0.014, -0.014, -0.016, 0.150, 0.151, 0.151, 0.148, 0.162, 0.732
Atom 4, 0.016, -0.013, -0.014, -0.016, 0.156, 0.160, 0.139, 0.150, 0.163, 0.741
Atom 5, 0.015, -0.013, -0.014, -0.017, 0.153, 0.146, 0.156, 0.152, 0.166, 0.744
Atom 6, 0.015, -0.013, -0.014, -0.018, 0.153, 0.147, 0.153, 0.151, 0.173, 0.747
Atom 7, 0.015, -0.013, -0.010, -0.015, 0.152, 0.108, 0.141, 0.148, 0.197, 0.724
Atom 8, 0.014, -0.012, -0.009, -0.012, 0.144, 0.093, 0.129, 0.144, 0.160, 0.652
Atom 9, 0.015, -0.010, -0.010, -0.013, 0.149, 0.117, 0.123, 0.146, 0.193, 0.708
Atom 10, 0.015, -0.011, -0.010, -0.015, 0.147, 0.128, 0.136, 0.143, 0.183, 0.717
Atom 11, 0.013, -0.012, -0.012, -0.012, 0.145, 0.145, 0.105, 0.145, 0.167, 0.685
Atom 12, 0.013, -0.011, -0.012, -0.014, 0.140, 0.145, 0.149, 0.146, 0.178, 0.735
Atom 13, 0.004, -0.014, -0.009, -0.004, 0.109, 0.081, 0.066, 0.119, 0.089, 0.440
Atom 14, 0.007, -0.016, -0.011, -0.008, 0.114, 0.081, 0.070, 0.137, 0.163, 0.536
Atom 15, -0.001, -0.011, -0.017, -0.006, 0.129, 0.035, 0.047, 0.104, 0.127, 0.407
Atom 16, 0.016, -0.012, -0.013, -0.006, 0.171, 0.134, 0.124, 0.153, 0.167, 0.734
Atom 17, 0.017, -0.013, -0.013, -0.006, 0.160, 0.134, 0.123, 0.161, 0.168, 0.730
Atom 18, 0.018, -0.014, -0.014, -0.008, 0.178, 0.124, 0.137, 0.158, 0.175, 0.755
Atom 19, 0.011, 0.013, 0.031, 0.008, -0.000, 0.000, 0.000, -0.000, -0.000, 0.064
Atom 20, 0.001, 0.005, -0.000, 0.007, 0.000, 0.000, 0.000, -0.000, 0.000, 0.013
Atom 21, -0.001, 0.000, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.001
Atom 22, 0.002, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.002
Atom 23, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000
Atom 24, 0.014, -0.015, -0.014, -0.013, 0.160, 0.114, 0.111, 0.143, 0.213, 0.712
Atom 25, 0.013, -0.015, -0.014, -0.013, 0.157, 0.113, 0.123, 0.141, 0.215, 0.720

Atom 26, 0.013, -0.015, -0.017, -0.012, 0.159, 0.113, 0.110, 0.143, 0.205, 0.698
Atom 27, 0.010, -0.014, -0.016, -0.012, 0.160, 0.109, 0.117, 0.144, 0.198, 0.695
Atom 28, 0.014, -0.014, -0.016, -0.012, 0.161, 0.119, 0.119, 0.144, 0.212, 0.726
Atom 29, 0.011, -0.013, -0.015, -0.010, 0.157, 0.118, 0.112, 0.145, 0.214, 0.720
total spin= 16.5729103278445

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.269, 0.332, 0.332, 0.337, 1.742, 1.772, 1.771, 1.745, 1.710, 10.009
Atom 2, 0.271, 0.330, 0.332, 0.332, 1.742, 1.765, 1.783, 1.741, 1.715, 10.010
Atom 3, 0.268, 0.330, 0.331, 0.334, 1.748, 1.763, 1.766, 1.745, 1.711, 9.996
Atom 4, 0.271, 0.331, 0.331, 0.336, 1.743, 1.756, 1.773, 1.742, 1.713, 9.997
Atom 5, 0.272, 0.331, 0.332, 0.337, 1.746, 1.764, 1.759, 1.742, 1.712, 9.995
Atom 6, 0.272, 0.332, 0.331, 0.336, 1.746, 1.766, 1.760, 1.741, 1.709, 9.992
Atom 7, 0.278, 0.329, 0.331, 0.333, 1.740, 1.788, 1.775, 1.749, 1.699, 10.022
Atom 8, 0.266, 0.328, 0.329, 0.336, 1.745, 1.785, 1.771, 1.747, 1.706, 10.014
Atom 9, 0.285, 0.329, 0.327, 0.326, 1.744, 1.776, 1.779, 1.742, 1.699, 10.007
Atom 10, 0.277, 0.329, 0.328, 0.332, 1.744, 1.780, 1.774, 1.746, 1.702, 10.012
Atom 11, 0.269, 0.330, 0.330, 0.336, 1.749, 1.762, 1.779, 1.744, 1.700, 9.999
Atom 12, 0.260, 0.334, 0.336, 0.349, 1.755, 1.767, 1.761, 1.749, 1.703, 10.016
Atom 13, 0.318, 0.284, 0.299, 0.231, 1.752, 1.734, 1.817, 1.748, 1.729, 9.911
Atom 14, 0.362, 0.329, 0.335, 0.237, 1.754, 1.803, 1.832, 1.740, 1.724, 10.115
Atom 15, 0.340, 0.309, 0.330, 0.293, 1.753, 1.893, 1.800, 1.749, 1.635, 10.100
Atom 16, 0.389, 0.311, 0.289, 0.161, 1.716, 1.800, 1.800, 1.733, 1.756, 9.955
Atom 17, 0.411, 0.289, 0.306, 0.161, 1.715, 1.791, 1.808, 1.733, 1.745, 9.959
Atom 18, 0.419, 0.312, 0.299, 0.171, 1.707, 1.801, 1.792, 1.729, 1.739, 9.969
Atom 19, 1.335, 0.908, 1.026, 0.958, 0.008, 0.006, 0.009, 0.009, 0.008, 4.268
Atom 20, 1.274, 0.944, 1.064, 0.941, 0.007, 0.007, 0.006, 0.007, 0.005, 4.254
Atom 21, 0.800, 0.004, 0.008, 0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.816
Atom 22, 0.818, 0.004, 0.006, 0.006, 0.000, 0.000, 0.000, 0.000, 0.000, 0.833
Atom 23, 0.769, 0.005, 0.007, 0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.787
Atom 24, 0.441, 0.299, 0.300, 0.164, 1.727, 1.805, 1.811, 1.732, 1.707, 9.985
Atom 25, 0.440, 0.300, 0.300, 0.165, 1.728, 1.804, 1.796, 1.732, 1.700, 9.965
Atom 26, 0.442, 0.299, 0.298, 0.166, 1.727, 1.805, 1.806, 1.730, 1.709, 9.982
Atom 27, 0.440, 0.300, 0.299, 0.166, 1.725, 1.806, 1.800, 1.731, 1.716, 9.985
Atom 28, 0.442, 0.301, 0.298, 0.166, 1.728, 1.801, 1.799, 1.732, 1.707, 9.974
Atom 29, 0.440, 0.302, 0.299, 0.167, 1.727, 1.799, 1.805, 1.731, 1.707, 9.977

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.156, -3.917, -3.898, -4.099, -2.078, -1.811, -1.792, -2.069, -2.202, -2.192
Atom 2, -5.175, -3.908, -3.889, -4.089, -2.078, -1.859, -1.811, -2.078, -2.202, -2.192
Atom 3, -5.147, -3.917, -3.908, -3.956, -2.078, -1.811, -1.811, -2.059, -2.202, -2.192
Atom 4, -5.137, -3.908, -3.917, -4.079, -2.088, -1.868, -1.840, -2.078, -2.231, -2.212
Atom 5, -5.166, -3.917, -3.908, -4.089, -2.078, -1.830, -1.859, -2.069, -2.221, -2.212
Atom 6, -5.166, -3.908, -3.908, -4.070, -2.088, -1.821, -1.840, -2.069, -2.221, -2.212
Atom 7, -5.166, -3.879, -3.860, -3.975, -2.059, -1.754, -1.792, -2.021, -2.183, -2.173
Atom 8, -5.185, -3.956, -3.898, -3.870, -2.002, -1.668, -1.725, -1.983, -2.192, -2.135
Atom 9, -5.156, -3.832, -3.813, -3.984, -2.040, -1.716, -1.725, -2.040, -2.154, -2.154
Atom 10, -5.195, -3.879, -3.841, -3.975, -2.049, -1.706, -1.764, -2.040, -2.154, -2.154
Atom 11, -5.156, -3.898, -3.927, -3.975, -2.021, -1.754, -1.735, -2.021, -2.202, -2.164
Atom 12, -5.471, -3.927, -3.946, -4.079, -2.078, -1.887, -1.907, -2.059, -2.240, -2.231
Atom 13, -4.537, -3.174, -3.250, -2.717, -1.926, -1.716, -1.573, -1.992, -2.059, -1.954
Atom 14, -4.994, -3.126, -3.441, -4.318, -1.973, -1.687, -1.659, -1.973, -2.021, -1.983
Atom 15, -5.595, -3.841, -3.365, -3.612, -1.992, -1.573, -1.849, -2.021, -2.640, -2.088
Atom 16, -4.404, -3.184, -3.508, -2.516, -1.897, -1.420, -1.525, -1.868, -1.602, -1.745

Atom 17, -4.346, -3.346, -3.041, -2.383, -2.002, -1.535, -1.373, -1.878, -1.592, -1.735
Atom 18, -4.203, -2.860, -3.069, -2.183, -2.049, -1.497, -1.497, -1.992, -1.592, -1.802
Atom 19, -15.173, -6.576, -6.357, -5.433, -5.461, -2.183, -3.288, -6.224, -3.060, -6.881
Atom 20, -15.173, -5.461, -6.319, -4.299, -3.593, -3.241, -7.225, -6.500, -5.328, -6.881
Atom 21, -6.586, -5.385, -6.338, -3.927, -15.554, -15.554, -15.554, -15.554, -15.554, -6.586
Atom 22, -7.644, -6.167, -6.758, -6.691, -15.554, -15.554, -15.554, -15.554, -15.554, -7.644
Atom 23, -7.672, -6.462, -5.566, -6.605, -15.554, -15.554, -15.554, -15.554, -15.554, -7.672
Atom 24, -4.203, -3.203, -3.203, -1.811, -1.916, -1.506, -1.497, -1.897, -1.621, -1.725
Atom 25, -4.213, -3.203, -3.203, -1.802, -1.916, -1.506, -1.506, -1.897, -1.611, -1.725
Atom 26, -4.184, -3.212, -3.231, -1.792, -1.907, -1.497, -1.487, -1.897, -1.602, -1.716
Atom 27, -4.184, -3.193, -3.212, -1.783, -1.916, -1.487, -1.487, -1.897, -1.602, -1.716
Atom 28, -4.175, -3.184, -3.222, -1.792, -1.916, -1.497, -1.506, -1.907, -1.611, -1.735
Atom 29, -4.242, -3.174, -3.203, -1.783, -1.916, -1.497, -1.497, -1.897, -1.611, -1.725

$CHCH_2$ adsorbed on Ni_{12} cluster

Ni1	10.0925099692	2.4969199999	4.0125600259
Ni2	5.7441400070	4.9857099924	4.0413200178
Ni3	7.1933299898	4.9836900148	2.0345799854
Ni4	9.3513299964	3.7377600246	2.0345799795
Ni5	9.3513299792	6.2296099648	2.0345799885
Ni6	11.5093300112	4.9836900916	2.0345800064
Ni7	10.0925100206	7.4806099973	4.0125599979
Ni8	12.2181400116	3.7397900176	4.0413200174
Ni9	12.2409300236	6.2427999608	4.0485900163
Ni10	7.8947400114	3.7422302035	4.1319600553
Ni11	7.9059701944	6.2556396732	4.0747999615
Ni12	10.1214197854	5.0065000595	4.1545999480
C13	8.5018045872	4.7715250929	5.7600860543
C14	9.4371247643	4.3420404693	6.6467507568
H15	9.9764657596	3.4059918008	6.5086657589
H16	9.6629006370	4.8730166805	7.5736128898
H17	8.0212353761	5.7024526220	6.1292584165

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000074 0.000044 0.000037
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	22.14	22.77	27.07	208.10	235.24	395.91
mode:	7	8	9	10	11	12
temp. (K):	508.29	599.09	1050.56	1456.65	1478.42	1548.68
mode:	13	14	15	16	17	18
temp. (K):	1878.70	2048.73	2296.15	4213.00	4506.52	4636.95

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 26.959 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

U	Cv	S	H	G	ln(Q)

trans.	0.889	2.981	60.853	1.481	-16.662	28.12233
rot.	0.889	2.981	50.683	0.889	-14.222	24.00470
vib.	3.335	16.558	30.444	3.335	-5.742	9.69153
elec.	0.000	0.000	4.132	0.000	-1.232	2.07944
total	5.112	22.520	146.112	5.705	-37.859	63.89800

Total internal energy, Utot (SCFE + ZPE + U): -2109.710359 hartrees
Total enthalpy, Htot (Utot + pV): -2109.709415 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2109.778837 hartrees

$CHCH_2$ gas

$CHCH_2$ gas in periodic cell

5 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.23681 1.08034 1.13028
C 2.23885 1.22114 2.43355
H 1.79522 2.09230 2.92436
H 2.68795 0.46768 3.09586
H 2.58156 0.35573 0.39825

FINAL RELAXED ENERGY = -26.1058100013

$CHCH_2$ gas in non-periodic calculation

C1	8.6206640259	4.9402293020	5.5827054814
C2	9.7564430321	4.6433257708	6.1637347328
H3	10.2077196146	3.6545881048	6.0828516380
H4	10.3137691722	5.3735410562	6.7598020339
H5	7.9643850848	5.7966768557	5.4932363185

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 11.288678 1.558314 1.369294
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 1038.70 1174.72 1327.14 1525.99 2017.96 2402.89
mode: 7 8 9
temp. (K): 4413.57 4553.06 4683.04

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 22.989 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.818	1.481	-9.198	15.52418
rot.	0.889	2.981	17.940	0.889	-4.460	7.52791

vib.	0.167	2.343	0.700	0.167	-0.041	0.07001
elec.	0.000	0.000	1.377	0.000	-0.411	0.69315
total	1.945	8.305	55.835	2.537	-14.110	23.81525

Total internal energy, Utot (SCFE + ZPE + U): -77.864658 hartrees
Total enthalpy, Htot (Utot + pV): -77.863714 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -77.890243 hartrees

CHCH binding at fcc-hcp site

CHCH adsorbed in periodic cell

28 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000
Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.40701 -0.00533 4.03117
Ni 1.44625 2.49472 4.11315
Ni 3.58677 1.18686 4.10113
Ni 3.59510 3.79779 4.10165
Ni 5.77846 0.00558 4.04072
Ni 5.73991 2.48780 4.10816
C 4.28635 2.49366 5.48913
C 2.88741 2.49126 5.49159
H 4.88205 2.49407 6.41045
H 2.29609 2.48767 6.41629
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2271.8548997880

Total electrons from output= 250
Spin up from output= 133.0000000000
Spin down from output= 117.0000000000
Fermi level up from output= -4.3198097378
Fermi level down from output= -4.418421677
# of atoms= 28

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.012, -0.017, 0.153, 0.152, 0.138, 0.154, 0.166, 0.737
Atom 2, 0.015, -0.013, -0.012, -0.017, 0.152, 0.136, 0.141, 0.152, 0.164, 0.717

Atom 3, 0.016, -0.012, -0.013, -0.016, 0.154, 0.143, 0.133, 0.150, 0.162, 0.716
Atom 4, 0.017, -0.013, -0.013, -0.016, 0.154, 0.145, 0.130, 0.152, 0.161, 0.716
Atom 5, 0.016, -0.013, -0.013, -0.018, 0.155, 0.164, 0.145, 0.153, 0.164, 0.753
Atom 6, 0.016, -0.013, -0.013, -0.015, 0.148, 0.151, 0.156, 0.152, 0.162, 0.744
Atom 7, 0.014, -0.013, -0.010, -0.013, 0.141, 0.119, 0.133, 0.145, 0.179, 0.696
Atom 8, 0.015, -0.010, -0.010, -0.012, 0.151, 0.123, 0.096, 0.144, 0.172, 0.669
Atom 9, 0.015, -0.011, -0.009, -0.012, 0.148, 0.096, 0.134, 0.142, 0.153, 0.657
Atom 10, 0.016, -0.012, -0.010, -0.013, 0.160, 0.104, 0.125, 0.150, 0.219, 0.739
Atom 11, 0.013, -0.011, -0.011, -0.014, 0.151, 0.136, 0.115, 0.144, 0.184, 0.708
Atom 12, 0.014, -0.011, -0.011, -0.013, 0.150, 0.132, 0.109, 0.144, 0.181, 0.695
Atom 13, 0.017, -0.011, -0.010, -0.007, 0.169, 0.128, 0.130, 0.154, 0.159, 0.729
Atom 14, 0.007, -0.011, -0.012, -0.007, 0.124, 0.067, 0.094, 0.125, 0.084, 0.471
Atom 15, -0.000, -0.010, -0.013, -0.006, 0.098, 0.098, 0.039, 0.106, 0.115, 0.426
Atom 16, -0.000, -0.010, -0.013, -0.006, 0.099, 0.098, 0.038, 0.106, 0.116, 0.427
Atom 17, 0.016, -0.010, -0.011, -0.007, 0.169, 0.119, 0.127, 0.158, 0.162, 0.724
Atom 18, 0.008, -0.010, -0.014, -0.006, 0.132, 0.083, 0.081, 0.119, 0.090, 0.482
Atom 19, 0.004, 0.003, 0.017, 0.006, -0.000, 0.000, 0.000, 0.000, -0.000, 0.030
Atom 20, 0.004, 0.005, 0.019, 0.008, -0.000, 0.000, 0.000, 0.000, -0.000, 0.036
Atom 21, -0.002, 0.000, 0.000, -0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.002
Atom 22, -0.003, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.003
Atom 23, 0.012, -0.014, -0.014, -0.012, 0.160, 0.113, 0.116, 0.147, 0.213, 0.721
Atom 24, 0.016, -0.014, -0.016, -0.011, 0.160, 0.117, 0.120, 0.146, 0.215, 0.732
Atom 25, 0.011, -0.015, -0.015, -0.013, 0.161, 0.113, 0.111, 0.145, 0.204, 0.701
Atom 26, 0.014, -0.013, -0.015, -0.012, 0.159, 0.113, 0.117, 0.144, 0.211, 0.718
Atom 27, 0.011, -0.014, -0.015, -0.012, 0.161, 0.114, 0.115, 0.148, 0.197, 0.705
Atom 28, 0.014, -0.014, -0.016, -0.013, 0.160, 0.116, 0.115, 0.146, 0.206, 0.713
total spin= 16.1586689293328

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.333, 0.334, 1.746, 1.763, 1.773, 1.745, 1.718, 10.016
Atom 2, 0.270, 0.331, 0.333, 0.335, 1.747, 1.770, 1.768, 1.748, 1.715, 10.018
Atom 3, 0.270, 0.333, 0.332, 0.335, 1.745, 1.770, 1.778, 1.749, 1.716, 10.028
Atom 4, 0.270, 0.331, 0.332, 0.333, 1.747, 1.768, 1.782, 1.747, 1.716, 10.026
Atom 5, 0.273, 0.332, 0.334, 0.336, 1.746, 1.755, 1.769, 1.747, 1.714, 10.004
Atom 6, 0.270, 0.332, 0.332, 0.336, 1.752, 1.762, 1.760, 1.748, 1.716, 10.008
Atom 7, 0.267, 0.330, 0.332, 0.341, 1.756, 1.782, 1.778, 1.751, 1.699, 10.037
Atom 8, 0.269, 0.325, 0.330, 0.334, 1.743, 1.777, 1.802, 1.747, 1.698, 10.025
Atom 9, 0.262, 0.330, 0.332, 0.337, 1.747, 1.790, 1.767, 1.752, 1.712, 10.030
Atom 10, 0.293, 0.325, 0.327, 0.324, 1.737, 1.788, 1.795, 1.748, 1.684, 10.022
Atom 11, 0.279, 0.329, 0.331, 0.333, 1.746, 1.776, 1.787, 1.746, 1.696, 10.023
Atom 12, 0.278, 0.327, 0.330, 0.333, 1.747, 1.775, 1.790, 1.747, 1.697, 10.025
Atom 13, 0.417, 0.311, 0.305, 0.164, 1.707, 1.793, 1.799, 1.728, 1.754, 9.977
Atom 14, 0.305, 0.348, 0.302, 0.217, 1.738, 1.849, 1.692, 1.739, 1.814, 10.002
Atom 15, 0.305, 0.302, 0.316, 0.244, 1.715, 1.770, 1.761, 1.798, 1.774, 9.984
Atom 16, 0.305, 0.304, 0.315, 0.244, 1.715, 1.770, 1.762, 1.798, 1.772, 9.985
Atom 17, 0.417, 0.309, 0.293, 0.163, 1.709, 1.802, 1.804, 1.725, 1.750, 9.972
Atom 18, 0.311, 0.330, 0.311, 0.222, 1.731, 1.827, 1.715, 1.747, 1.814, 10.006
Atom 19, 1.310, 0.897, 0.903, 1.056, 0.009, 0.003, 0.012, 0.007, 0.008, 4.205
Atom 20, 1.323, 0.905, 0.899, 1.047, 0.009, 0.003, 0.012, 0.007, 0.008, 4.213
Atom 21, 0.826, 0.005, 0.003, 0.008, 0.000, 0.000, 0.000, 0.000, 0.000, 0.842
Atom 22, 0.829, 0.005, 0.003, 0.008, 0.000, 0.000, 0.000, 0.000, 0.000, 0.845
Atom 23, 0.441, 0.301, 0.300, 0.166, 1.729, 1.805, 1.804, 1.734, 1.705, 9.984
Atom 24, 0.442, 0.301, 0.299, 0.166, 1.731, 1.804, 1.802, 1.734, 1.707, 9.985
Atom 25, 0.441, 0.300, 0.300, 0.165, 1.730, 1.805, 1.809, 1.735, 1.712, 9.997
Atom 26, 0.442, 0.301, 0.299, 0.166, 1.730, 1.804, 1.802, 1.735, 1.707, 9.986

Atom 27, 0.441, 0.301, 0.300, 0.166, 1.728, 1.804, 1.803, 1.734, 1.719, 9.996
Atom 28, 0.442, 0.301, 0.300, 0.166, 1.730, 1.803, 1.802, 1.734, 1.712, 9.990

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.147, -3.909, -3.889, -4.121, -2.100, -1.878, -1.858, -2.090, -2.235, -2.216
Atom 2, -5.156, -3.918, -3.899, -4.034, -2.081, -1.820, -1.829, -2.071, -2.226, -2.206
Atom 3, -5.137, -3.909, -3.909, -4.044, -2.090, -1.868, -1.829, -2.081, -2.226, -2.206
Atom 4, -5.147, -3.899, -3.899, -4.034, -2.100, -1.878, -1.839, -2.071, -2.226, -2.206
Atom 5, -5.176, -3.918, -3.889, -4.063, -2.110, -1.907, -1.858, -2.090, -2.255, -2.226
Atom 6, -5.118, -3.909, -3.909, -3.947, -2.081, -1.878, -1.878, -2.081, -2.226, -2.216
Atom 7, -5.417, -3.986, -3.967, -4.015, -2.061, -1.820, -1.829, -2.061, -2.235, -2.206
Atom 8, -5.137, -3.889, -3.860, -3.909, -2.023, -1.742, -1.684, -2.013, -2.216, -2.158
Atom 9, -5.263, -3.928, -3.870, -3.831, -2.023, -1.684, -1.752, -1.994, -2.177, -2.148
Atom 10, -5.147, -3.831, -3.812, -3.889, -2.061, -1.694, -1.703, -2.023, -2.177, -2.158
Atom 11, -5.369, -3.909, -3.889, -3.947, -2.061, -1.771, -1.742, -2.052, -2.197, -2.177
Atom 12, -5.359, -3.909, -3.860, -3.918, -2.042, -1.762, -1.733, -2.042, -2.187, -2.168
Atom 13, -4.247, -2.961, -3.125, -2.303, -2.013, -1.539, -1.491, -1.984, -1.578, -1.791
Atom 14, -5.234, -3.783, -3.667, -3.928, -2.100, -1.384, -1.762, -1.965, -1.674, -1.878
Atom 15, -5.456, -3.261, -3.560, -3.841, -2.100, -1.762, -1.965, -2.090, -2.042, -2.119
Atom 16, -5.456, -3.251, -3.570, -3.841, -2.100, -1.752, -1.955, -2.090, -2.052, -2.119
Atom 17, -4.228, -2.980, -3.222, -2.381, -1.955, -1.433, -1.462, -1.945, -1.587, -1.762
Atom 18, -5.195, -3.744, -3.512, -3.918, -2.090, -1.404, -1.713, -1.965, -1.665, -1.878
Atom 19, -15.505, -6.423, -5.446, -5.224, -3.619, -2.796, -4.063, -6.288, -3.096, -6.888
Atom 20, -15.515, -6.404, -5.456, -5.456, -3.570, -2.787, -3.909, -6.153, -3.164, -7.197
Atom 21, -8.290, -6.539, -5.853, -10.079, -15.911, -15.911, -15.911, -15.911, -15.911, -8.290
Atom 22, -8.300, -6.510, -5.872, -10.079, -15.911, -15.911, -15.911, -15.911, -15.911, -8.300
Atom 23, -4.208, -3.203, -3.212, -1.791, -1.926, -1.500, -1.500, -1.907, -1.636, -1.733
Atom 24, -4.208, -3.183, -3.222, -1.800, -1.926, -1.510, -1.520, -1.916, -1.645, -1.742
Atom 25, -4.199, -3.203, -3.203, -1.810, -1.926, -1.500, -1.500, -1.897, -1.626, -1.733
Atom 26, -4.208, -3.193, -3.212, -1.791, -1.926, -1.520, -1.500, -1.907, -1.636, -1.742
Atom 27, -4.189, -3.193, -3.203, -1.781, -1.936, -1.500, -1.500, -1.907, -1.616, -1.733
Atom 28, -4.199, -3.193, -3.222, -1.791, -1.926, -1.510, -1.510, -1.907, -1.626, -1.733

CHCH adsorbed on Ni_{12} cluster

Ni1	2.1579999995	1.2459199730	2.0345799937
Ni2	2.1579999919	3.7377600154	2.0345800052
Ni3	5.0353300220	1.2459199659	2.0345800095
Ni4	5.0353300061	3.7377600149	2.0345799995
Ni5	1.4070099975	-0.0053299929	4.0311700302
Ni6	5.7784600010	0.0055800058	4.0407200298
Ni7	1.4070099975	4.9783599945	4.0311700256
Ni8	5.7784600003	4.9892699966	4.0407200304
Ni9	1.4462501246	2.4947199855	4.1131499752
Ni10	3.5867699631	1.1868603231	4.1011299505
Ni11	3.5951000130	3.7977897110	4.1016500049
Ni12	5.7399098836	2.4878000072	4.1081599455
C13	4.1833086666	2.4780704574	5.6000327678
C14	2.8056489861	2.5018957063	5.6258784415
H15	4.7879568797	2.4779875365	6.5120462653
H16	2.2516221547	2.5051211659	6.5712504618

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000053 0.000051 0.000034

vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 17.98 20.86 23.58 27.16 29.06 29.51
mode: 7 8 9 10 11 12
temp. (K): 382.71 432.55 642.50 653.32 829.23 1226.20
mode: 13 14 15 16 17 18
temp. (K): 1448.97 1474.85 1735.16 1998.84 4463.01 4498.57

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 19.807 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.853	1.481	-16.662	28.12232
rot.	0.889	2.981	50.922	0.889	-14.294	24.12479
vib.	4.503	20.726	47.339	4.503	-9.611	16.22132
elec.	0.000	0.000	3.198	0.000	-0.954	1.60944
total	6.281	26.688	162.312	6.873	-41.520	70.07787

Total internal energy, Utot (SCFE + ZPE + U): -2109.104562 hartrees
Total enthalpy, Htot (Utot + pV): -2109.103618 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2109.180737 hartrees

CHCH gas

CHCH gas in periodic cell

4 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.15103 1.64744 1.64306
C 2.22753 0.75349 2.45547
H 2.08551 2.44319 0.92979
H 2.29317 -0.04166 3.16958

FINAL RELAXED ENERGY = -24.9611650922

CHCH gas in non-periodic calculation

C1	0.0000000000	0.0000000000	0.6025447304
C2	0.0000000000	0.0000000000	-0.6025447304
H3	0.0000000000	0.0000000000	1.6683156714
H4	0.0000000000	0.0000000000	-1.6683156714

Thermochemical properties at 1.0000 atm
rotational symmetry number: 2
rotational temperatures (K): 1.693318 1.693318
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 902.78 902.79 1122.20 1122.21 3004.18 4957.15

mode: 7
temp. (K): 5096.94

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 16.999 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.704	1.481	-9.164	15.46717
rot.	0.592	1.987	10.885	0.592	-2.653	4.47776
vib.	0.289	3.325	1.259	0.289	-0.087	0.14623
elec.	0.000	0.000	0.000	0.000	0.000	0.00000
total	1.770	8.293	47.849	2.362	-11.904	20.09116

Total internal energy, Utot (SCFE + ZPE + U): -77.297781 hartrees
Total enthalpy, Htot (Utot + pV): -77.296837 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -77.319571 hartrees

CCH binding at fcc-hcp site

CCH adsorbed in periodic cell

27 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni	0.00000	0.00000	0.00000
Ni	0.00000	2.49184	0.00000
Ni	2.15800	1.24592	0.00000
Ni	2.15800	3.73776	0.00000
Ni	4.31600	0.00000	0.00000
Ni	4.31600	2.49184	0.00000
Ni	0.71933	1.24592	2.03458
Ni	0.71933	3.73776	2.03458
Ni	2.87733	0.00000	2.03458
Ni	2.87733	2.49184	2.03458
Ni	5.03533	1.24592	2.03458
Ni	5.03533	3.73776	2.03458
Ni	1.41109	-0.00544	4.04226
Ni	1.41480	2.49739	4.16145
Ni	3.62353	1.18300	4.06188
Ni	3.62805	3.80172	4.06117
Ni	5.78924	0.00027	4.04564
Ni	5.73728	2.49056	4.13935
C	2.86000	2.49466	5.30009
C	4.19371	2.49200	5.57003
H	4.74240	2.49239	6.51450
Ni	1.43867	0.00000	-2.03458
Ni	1.43867	2.49184	-2.03458
Ni	3.59667	1.24592	-2.03458
Ni	3.59667	3.73776	-2.03458

Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2270.6221350203

Total electrons from output= 249
Spin up from output= 132.5000000000
Spin down from output= 116.5000000000
Fermi level up from output= -4.6573188956
Fermi level down from output= -4.7491825564
# of atoms= 27

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.017, -0.013, -0.013, -0.018, 0.155, 0.141, 0.145, 0.154, 0.167, 0.735
Atom 2, 0.015, -0.014, -0.012, -0.019, 0.154, 0.139, 0.154, 0.149, 0.164, 0.730
Atom 3, 0.016, -0.013, -0.014, -0.016, 0.155, 0.142, 0.133, 0.151, 0.160, 0.714
Atom 4, 0.016, -0.013, -0.014, -0.016, 0.156, 0.146, 0.136, 0.153, 0.161, 0.724
Atom 5, 0.015, -0.013, -0.013, -0.018, 0.155, 0.166, 0.142, 0.154, 0.166, 0.754
Atom 6, 0.015, -0.013, -0.014, -0.016, 0.149, 0.152, 0.152, 0.153, 0.162, 0.741
Atom 7, 0.013, -0.013, -0.011, -0.012, 0.139, 0.122, 0.127, 0.148, 0.175, 0.688
Atom 8, 0.014, -0.010, -0.010, -0.011, 0.149, 0.127, 0.093, 0.146, 0.177, 0.673
Atom 9, 0.015, -0.010, -0.009, -0.014, 0.136, 0.100, 0.140, 0.143, 0.159, 0.659
Atom 10, 0.017, -0.011, -0.010, -0.013, 0.159, 0.107, 0.117, 0.154, 0.214, 0.734
Atom 11, 0.014, -0.012, -0.010, -0.015, 0.150, 0.138, 0.125, 0.144, 0.189, 0.724
Atom 12, 0.014, -0.012, -0.011, -0.014, 0.147, 0.135, 0.119, 0.143, 0.190, 0.711
Atom 13, 0.017, -0.011, -0.011, -0.006, 0.167, 0.147, 0.132, 0.151, 0.176, 0.762
Atom 14, -0.002, -0.008, -0.013, -0.006, 0.099, 0.044, 0.124, 0.107, 0.097, 0.442
Atom 15, 0.002, -0.014, -0.012, -0.005, 0.086, 0.108, 0.048, 0.115, 0.111, 0.438
Atom 16, 0.002, -0.015, -0.013, -0.006, 0.092, 0.110, 0.047, 0.118, 0.114, 0.449
Atom 17, 0.019, -0.012, -0.013, -0.008, 0.184, 0.125, 0.140, 0.161, 0.163, 0.758
Atom 18, 0.006, -0.012, -0.014, -0.008, 0.142, 0.094, 0.092, 0.135, 0.090, 0.525
Atom 19, 0.026, 0.026, 0.013, 0.004, -0.000, -0.000, 0.000, 0.000, -0.000, 0.068
Atom 20, 0.007, 0.003, 0.030, 0.006, -0.000, 0.000, -0.000, 0.000, -0.000, 0.046
Atom 21, -0.005, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, -0.004
Atom 22, 0.013, -0.015, -0.014, -0.011, 0.159, 0.109, 0.116, 0.146, 0.219, 0.722
Atom 23, 0.016, -0.016, -0.016, -0.011, 0.160, 0.114, 0.119, 0.145, 0.219, 0.730
Atom 24, 0.008, -0.013, -0.015, -0.016, 0.160, 0.113, 0.113, 0.145, 0.201, 0.695
Atom 25, 0.013, -0.012, -0.017, -0.013, 0.160, 0.116, 0.121, 0.144, 0.215, 0.728
Atom 26, 0.012, -0.013, -0.016, -0.013, 0.162, 0.117, 0.115, 0.146, 0.201, 0.711
Atom 27, 0.012, -0.014, -0.016, -0.014, 0.159, 0.119, 0.116, 0.145, 0.209, 0.718
total spin= 16.372456250264

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.271, 0.331, 0.332, 0.333, 1.744, 1.770, 1.771, 1.742, 1.715, 10.010
Atom 2, 0.271, 0.331, 0.333, 0.334, 1.746, 1.768, 1.762, 1.746, 1.713, 10.003
Atom 3, 0.270, 0.332, 0.331, 0.335, 1.744, 1.768, 1.775, 1.747, 1.715, 10.018
Atom 4, 0.270, 0.331, 0.331, 0.333, 1.744, 1.768, 1.773, 1.746, 1.714, 10.010
Atom 5, 0.273, 0.332, 0.333, 0.337, 1.744, 1.752, 1.770, 1.744, 1.712, 9.996
Atom 6, 0.270, 0.332, 0.332, 0.336, 1.749, 1.761, 1.761, 1.744, 1.714, 9.999
Atom 7, 0.272, 0.330, 0.332, 0.338, 1.752, 1.773, 1.774, 1.747, 1.702, 10.019
Atom 8, 0.278, 0.324, 0.330, 0.328, 1.742, 1.771, 1.797, 1.743, 1.697, 10.011
Atom 9, 0.254, 0.335, 0.333, 0.339, 1.753, 1.788, 1.755, 1.751, 1.717, 10.024
Atom 10, 0.288, 0.327, 0.325, 0.312, 1.736, 1.783, 1.796, 1.744, 1.683, 9.993
Atom 11, 0.275, 0.329, 0.331, 0.331, 1.746, 1.774, 1.780, 1.745, 1.695, 10.006

Atom 12, 0.274, 0.327, 0.330, 0.333, 1.748, 1.770, 1.786, 1.747, 1.694, 10.009
Atom 13, 0.410, 0.297, 0.292, 0.155, 1.712, 1.786, 1.795, 1.733, 1.741, 9.922
Atom 14, 0.321, 0.377, 0.294, 0.273, 1.756, 1.873, 1.678, 1.732, 1.726, 10.029
Atom 15, 0.306, 0.305, 0.337, 0.254, 1.740, 1.748, 1.796, 1.774, 1.775, 10.035
Atom 16, 0.304, 0.308, 0.337, 0.255, 1.738, 1.749, 1.796, 1.774, 1.773, 10.033
Atom 17, 0.401, 0.314, 0.291, 0.161, 1.711, 1.800, 1.794, 1.725, 1.747, 9.944
Atom 18, 0.353, 0.309, 0.304, 0.206, 1.721, 1.829, 1.731, 1.744, 1.810, 10.005
Atom 19, 1.463, 0.874, 0.794, 0.800, 0.013, 0.005, 0.011, 0.009, 0.008, 3.977
Atom 20, 1.352, 0.879, 0.910, 1.026, 0.008, 0.003, 0.011, 0.006, 0.008, 4.202
Atom 21, 0.806, 0.005, 0.003, 0.008, 0.000, 0.000, 0.000, 0.000, 0.000, 0.822
Atom 22, 0.441, 0.300, 0.299, 0.167, 1.727, 1.808, 1.800, 1.733, 1.700, 9.974
Atom 23, 0.442, 0.300, 0.298, 0.166, 1.727, 1.808, 1.800, 1.733, 1.702, 9.975
Atom 24, 0.439, 0.301, 0.299, 0.163, 1.728, 1.804, 1.805, 1.734, 1.710, 9.983
Atom 25, 0.441, 0.302, 0.299, 0.164, 1.729, 1.801, 1.798, 1.733, 1.702, 9.969
Atom 26, 0.441, 0.301, 0.299, 0.166, 1.727, 1.800, 1.802, 1.731, 1.714, 9.981
Atom 27, 0.441, 0.300, 0.300, 0.165, 1.729, 1.799, 1.800, 1.731, 1.709, 9.974

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.130, -3.915, -3.905, -4.128, -2.096, -1.853, -1.863, -2.087, -2.223, -2.213
Atom 2, -5.130, -3.924, -3.915, -4.041, -2.077, -1.824, -1.843, -2.077, -2.223, -2.213
Atom 3, -5.149, -3.915, -3.924, -4.031, -2.087, -1.853, -1.824, -2.067, -2.223, -2.203
Atom 4, -5.149, -3.915, -3.905, -4.051, -2.096, -1.873, -1.853, -2.067, -2.223, -2.203
Atom 5, -5.179, -3.915, -3.885, -4.070, -2.106, -1.902, -1.863, -2.087, -2.252, -2.223
Atom 6, -5.111, -3.905, -3.895, -3.963, -2.087, -1.873, -1.873, -2.077, -2.232, -2.213
Atom 7, -5.519, -3.973, -3.895, -3.944, -2.067, -1.795, -1.814, -2.057, -2.223, -2.194
Atom 8, -5.111, -3.866, -3.817, -3.905, -2.009, -1.737, -1.659, -2.019, -2.203, -2.145
Atom 9, -5.451, -3.895, -3.895, -3.846, -2.019, -1.727, -1.843, -2.009, -2.174, -2.155
Atom 10, -5.091, -3.788, -3.788, -3.876, -2.019, -1.678, -1.649, -2.009, -2.155, -2.135
Atom 11, -5.499, -3.983, -3.973, -4.031, -2.067, -1.756, -1.805, -2.038, -2.203, -2.184
Atom 12, -5.470, -3.944, -3.924, -3.983, -2.048, -1.766, -1.814, -2.019, -2.194, -2.174
Atom 13, -4.342, -3.244, -3.253, -2.407, -1.921, -1.503, -1.464, -1.882, -1.581, -1.756
Atom 14, -6.520, -4.090, -4.109, -3.030, -2.184, -1.455, -1.921, -2.057, -2.135, -2.048
Atom 15, -5.723, -3.331, -3.555, -3.876, -2.184, -1.950, -1.921, -2.164, -2.048, -2.194
Atom 16, -5.704, -3.351, -3.555, -3.866, -2.184, -1.960, -1.931, -2.155, -2.067, -2.194
Atom 17, -4.245, -3.010, -3.321, -2.407, -2.038, -1.474, -1.503, -1.999, -1.620, -1.805
Atom 18, -4.498, -3.496, -3.244, -3.691, -2.106, -1.348, -1.668, -1.931, -1.610, -1.824
Atom 19, -9.671, -6.394, -5.548, -4.926, -3.321, -2.806, -5.850, -6.462, -3.963, -6.122
Atom 20, -15.505, -6.209, -5.490, -6.530, -4.158, -3.253, -2.631, -6.734, -4.498, -6.559
Atom 21, -9.583, -6.462, -5.869, -9.622, -15.913, -15.913, -15.913, -15.913, -15.913, -9.583
Atom 22, -4.216, -3.214, -3.224, -1.795, -1.921, -1.503, -1.503, -1.902, -1.630, -1.737
Atom 23, -4.216, -3.205, -3.214, -1.795, -1.931, -1.503, -1.513, -1.912, -1.639, -1.746
Atom 24, -4.197, -3.185, -3.214, -1.834, -1.921, -1.493, -1.503, -1.902, -1.620, -1.727
Atom 25, -4.197, -3.185, -3.224, -1.805, -1.921, -1.513, -1.503, -1.902, -1.630, -1.737
Atom 26, -4.187, -3.195, -3.214, -1.785, -1.931, -1.503, -1.503, -1.902, -1.620, -1.737
Atom 27, -4.206, -3.214, -3.224, -1.795, -1.921, -1.513, -1.513, -1.902, -1.630, -1.737

CCH adsorbed on Ni_{12} cluster

Ni1	2.1579999461	1.2459198972	2.0345800323
Ni2	2.1579999566	3.7377600680	2.0345800206
Ni3	5.0353300133	1.2459199272	2.0345799796
Ni4	5.0353300854	3.7377600776	2.0345800305
Ni5	1.4110899909	-0.0054399775	4.0422600603
Ni6	5.7892399918	0.0002700138	4.0456400805
Ni7	1.4110899807	4.9782499681	4.0422600785

Ni8 5.7892399910 4.9839499731 4.0456400756
Ni9 1.4148002772 2.4973900053 4.1614499339
Ni10 3.6235301421 1.1830007100 4.0618798909
Ni11 3.6280500493 3.8017193745 4.0611698743
Ni12 5.7372795757 2.4905599626 4.1393499431
C13 2.7338977024 2.5068375780 5.5283143339
C14 3.9141829262 2.5192274456 5.9979220843
H15 4.6373837943 2.5200235220 6.7907973756
Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000053 0.000051 0.000034
vibrational temperatures:
mode: 1 2 3 4 5 6
temp. (K): 16.91 19.06 22.38 25.27 27.70 28.28
mode: 7 8 9 10 11 12
temp. (K): 323.68 374.38 549.19 670.39 778.95 1267.24
mode: 13 14 15
temp. (K): 1284.47 2662.14 4937.11

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 12.904 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.853	1.481	-16.662	28.12231
rot.	0.889	2.981	50.931	0.889	-14.296	24.12946
vib.	4.600	20.517	48.767	4.600	-9.940	16.77719
elec.	0.000	0.000	4.132	0.000	-1.232	2.07944
total	6.377	26.478	164.683	6.970	-42.131	71.10840

Total internal energy, Utot (SCFE + ZPE + U): -2108.505648 hartrees
Total enthalpy, Htot (Utot + pV): -2108.504704 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2108.582951 hartrees

CCH gas

CCH gas in periodic cell

3 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.15885 1.25144 1.60239
C 2.26914 1.24124 0.39114
H 2.18809 1.15169 2.66852

FINAL RELAXED ENERGY = -23.5278413461

CHCH gas in non-periodic calculation

C1 0.0000000000 0.0000000000 -0.6721674064

C2 0.0000000000 0.0000000000 0.5373782840
H3 0.0000000000 0.0000000000 1.6049109891

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 2.112212 2.112212
2 vibrational frequencies below 10.0 cm-1 not included in zero-point energy or thermochemical analysis. Set freqcut to change the frequency cutoff value.

vibrational temperatures:
mode: 3 4
temp. (K): 3033.59 5007.56

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 7.990 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.587	1.481	-9.129	15.40791
rot.	0.592	1.987	11.824	0.592	-2.933	4.94986
vib.	0.000	0.008	0.001	0.000	0.000	0.00004
elec.	0.000	0.000	1.377	0.000	-0.411	0.69315
total	1.481	4.976	48.789	2.074	-12.472	21.05095

Total internal energy, Utot (SCFE + ZPE + U): -76.588421 hartrees
Total enthalpy, Htot (Utot + pV): -76.587477 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -76.610658 hartrees

C_2 binding at fcc-hcp site

C_2 adsorbed in periodic cell

26 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

Ni 0.00000 0.00000 0.00000
Ni 0.00000 2.49184 0.00000
Ni 2.15800 1.24592 0.00000
Ni 2.15800 3.73776 0.00000
Ni 4.31600 0.00000 0.00000
Ni 4.31600 2.49184 0.00000
Ni 0.71933 1.24592 2.03458
Ni 0.71933 3.73776 2.03458
Ni 2.87733 0.00000 2.03458
Ni 2.87733 2.49184 2.03458
Ni 5.03533 1.24592 2.03458
Ni 5.03533 3.73776 2.03458
Ni 1.42010 -0.00451 4.04129
Ni 1.45499 2.49329 4.22899
Ni 3.60631 1.17360 4.01992

Ni 3.60998 3.80751 4.02134
Ni 5.80269 0.00450 4.05641
Ni 5.77899 2.48603 4.22023
C 4.29272 2.49139 5.39311
C 2.95563 2.48813 5.39423
Ni 1.43867 0.00000 -2.03458
Ni 1.43867 2.49184 -2.03458
Ni 3.59667 1.24592 -2.03458
Ni 3.59667 3.73776 -2.03458
Ni 5.75467 0.00000 -2.03458
Ni 5.75467 2.49184 -2.03458

FINAL RELAXED ENERGY = -2269.3718250060

Total electrons from output= 248
Spin up from output= 132.5000000000
Spin down from output= 115.5000000000
Fermi level up from output= -5.284813549
Fermi level down from output= -5.4077111272
# of atoms= 26

spin:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.018, -0.013, -0.012, -0.017, 0.159, 0.147, 0.152, 0.158, 0.170, 0.760
Atom 2, 0.016, -0.013, -0.011, -0.019, 0.157, 0.143, 0.155, 0.154, 0.166, 0.748
Atom 3, 0.016, -0.012, -0.013, -0.014, 0.159, 0.139, 0.141, 0.156, 0.163, 0.736
Atom 4, 0.017, -0.013, -0.013, -0.015, 0.159, 0.145, 0.134, 0.158, 0.162, 0.734
Atom 5, 0.015, -0.013, -0.011, -0.017, 0.161, 0.162, 0.147, 0.157, 0.166, 0.768
Atom 6, 0.017, -0.013, -0.012, -0.016, 0.154, 0.158, 0.160, 0.156, 0.164, 0.767
Atom 7, 0.013, -0.011, -0.011, -0.011, 0.143, 0.129, 0.137, 0.154, 0.177, 0.720
Atom 8, 0.012, -0.008, -0.010, -0.009, 0.153, 0.137, 0.104, 0.153, 0.172, 0.702
Atom 9, 0.017, -0.010, -0.009, -0.014, 0.137, 0.096, 0.146, 0.152, 0.161, 0.675
Atom 10, 0.016, -0.011, -0.010, -0.012, 0.159, 0.110, 0.122, 0.158, 0.221, 0.752
Atom 11, 0.015, -0.012, -0.011, -0.015, 0.156, 0.132, 0.130, 0.143, 0.195, 0.735
Atom 12, 0.015, -0.012, -0.011, -0.014, 0.154, 0.132, 0.129, 0.142, 0.198, 0.732
Atom 13, 0.017, -0.012, -0.013, -0.008, 0.188, 0.159, 0.153, 0.154, 0.193, 0.832
Atom 14, 0.002, -0.010, -0.014, -0.006, 0.133, 0.057, 0.171, 0.131, 0.140, 0.604
Atom 15, 0.007, -0.017, -0.012, -0.004, 0.097, 0.133, 0.065, 0.171, 0.112, 0.553
Atom 16, 0.007, -0.017, -0.012, -0.004, 0.096, 0.135, 0.065, 0.171, 0.112, 0.552
Atom 17, 0.016, -0.011, -0.013, -0.007, 0.188, 0.137, 0.143, 0.158, 0.193, 0.804
Atom 18, 0.002, -0.010, -0.015, -0.006, 0.137, 0.066, 0.146, 0.120, 0.135, 0.574
Atom 19, 0.038, 0.047, 0.025, 0.037, -0.000, -0.000, 0.000, 0.001, -0.000, 0.148
Atom 20, 0.044, 0.051, 0.027, 0.044, -0.000, -0.000, -0.000, 0.001, -0.000, 0.168
Atom 21, 0.013, -0.011, -0.014, -0.011, 0.162, 0.110, 0.113, 0.150, 0.217, 0.730
Atom 22, 0.017, -0.013, -0.016, -0.009, 0.164, 0.118, 0.120, 0.149, 0.224, 0.755
Atom 23, 0.010, -0.012, -0.014, -0.015, 0.164, 0.119, 0.112, 0.148, 0.205, 0.717
Atom 24, 0.014, -0.010, -0.016, -0.013, 0.162, 0.120, 0.121, 0.148, 0.222, 0.747
Atom 25, 0.014, -0.013, -0.014, -0.012, 0.165, 0.118, 0.117, 0.151, 0.206, 0.732
Atom 26, 0.015, -0.014, -0.014, -0.012, 0.163, 0.120, 0.118, 0.148, 0.215, 0.739
total spin= 17.4833242972204

CHARGES:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, 0.272, 0.332, 0.333, 0.335, 1.743, 1.766, 1.767, 1.744, 1.716, 10.008
Atom 2, 0.271, 0.332, 0.334, 0.334, 1.746, 1.766, 1.762, 1.749, 1.715, 10.008
Atom 3, 0.271, 0.333, 0.333, 0.336, 1.743, 1.773, 1.771, 1.748, 1.715, 10.023

Atom 4, 0.270, 0.332, 0.333, 0.334, 1.743, 1.770, 1.776, 1.745, 1.717, 10.019
Atom 5, 0.274, 0.332, 0.335, 0.338, 1.741, 1.753, 1.772, 1.746, 1.713, 10.005
Atom 6, 0.271, 0.332, 0.333, 0.336, 1.748, 1.760, 1.763, 1.747, 1.715, 10.003
Atom 7, 0.281, 0.333, 0.331, 0.334, 1.751, 1.773, 1.767, 1.748, 1.701, 10.019
Atom 8, 0.291, 0.327, 0.327, 0.320, 1.741, 1.770, 1.787, 1.742, 1.701, 10.006
Atom 9, 0.239, 0.337, 0.333, 0.343, 1.756, 1.801, 1.754, 1.749, 1.717, 10.029
Atom 10, 0.289, 0.327, 0.329, 0.322, 1.739, 1.783, 1.794, 1.747, 1.683, 10.012
Atom 11, 0.281, 0.330, 0.328, 0.326, 1.742, 1.781, 1.778, 1.749, 1.693, 10.010
Atom 12, 0.280, 0.328, 0.327, 0.326, 1.745, 1.777, 1.779, 1.751, 1.691, 10.003
Atom 13, 0.394, 0.300, 0.305, 0.152, 1.713, 1.780, 1.784, 1.741, 1.730, 9.898
Atom 14, 0.370, 0.369, 0.285, 0.257, 1.738, 1.876, 1.682, 1.740, 1.733, 10.051
Atom 15, 0.298, 0.309, 0.347, 0.263, 1.770, 1.723, 1.811, 1.758, 1.784, 10.062
Atom 16, 0.300, 0.311, 0.347, 0.262, 1.770, 1.721, 1.811, 1.757, 1.783, 10.063
Atom 17, 0.397, 0.305, 0.284, 0.149, 1.716, 1.803, 1.795, 1.736, 1.726, 9.910
Atom 18, 0.374, 0.356, 0.292, 0.261, 1.734, 1.861, 1.699, 1.747, 1.731, 10.056
Atom 19, 1.495, 0.861, 0.767, 0.806, 0.011, 0.004, 0.011, 0.008, 0.006, 3.969
Atom 20, 1.507, 0.868, 0.768, 0.792, 0.011, 0.004, 0.011, 0.008, 0.006, 3.978
Atom 21, 0.442, 0.302, 0.299, 0.167, 1.728, 1.808, 1.803, 1.734, 1.704, 9.986
Atom 22, 0.444, 0.302, 0.299, 0.167, 1.728, 1.804, 1.800, 1.734, 1.700, 9.979
Atom 23, 0.440, 0.302, 0.300, 0.164, 1.728, 1.800, 1.808, 1.735, 1.713, 9.990
Atom 24, 0.441, 0.303, 0.300, 0.164, 1.729, 1.799, 1.800, 1.735, 1.698, 9.969
Atom 25, 0.443, 0.301, 0.300, 0.167, 1.726, 1.800, 1.802, 1.733, 1.712, 9.984
Atom 26, 0.443, 0.300, 0.301, 0.166, 1.728, 1.799, 1.800, 1.734, 1.705, 9.976

BAND CENTER:
Atom#, s, px, py, pz, dxy, dyz, dxz, dx2-y2, dr2-z2, total
Atom 1, -5.163, -3.917, -3.897, -4.121, -2.106, -1.901, -1.892, -2.096, -2.262, -2.232
Atom 2, -5.163, -3.926, -3.907, -4.082, -2.096, -1.853, -1.862, -2.096, -2.252, -2.223
Atom 3, -5.221, -3.936, -3.926, -4.043, -2.106, -1.862, -1.853, -2.086, -2.242, -2.223
Atom 4, -5.212, -3.926, -3.907, -4.063, -2.106, -1.872, -1.872, -2.077, -2.232, -2.213
Atom 5, -5.260, -3.917, -3.878, -4.121, -2.125, -1.940, -1.882, -2.106, -2.271, -2.242
Atom 6, -5.153, -3.926, -3.907, -3.975, -2.106, -1.892, -1.901, -2.096, -2.252, -2.232
Atom 7, -5.494, -3.926, -3.907, -3.907, -2.086, -1.785, -1.814, -2.067, -2.232, -2.203
Atom 8, -5.143, -3.790, -3.800, -3.761, -2.018, -1.707, -1.600, -2.018, -2.184, -2.125
Atom 9, -5.406, -3.926, -3.956, -3.858, -2.018, -1.755, -1.862, -2.028, -2.193, -2.184
Atom 10, -5.143, -3.780, -3.810, -3.897, -2.038, -1.755, -1.677, -2.047, -2.193, -2.174
Atom 11, -5.416, -3.917, -3.907, -3.956, -2.077, -1.716, -1.814, -2.038, -2.203, -2.193
Atom 12, -5.377, -3.946, -3.907, -3.936, -2.057, -1.707, -1.814, -2.009, -2.193, -2.174
Atom 13, -4.316, -3.216, -3.148, -2.515, -2.028, -1.590, -1.551, -1.950, -1.648, -1.833
Atom 14, -5.416, -3.771, -3.878, -3.518, -2.184, -1.356, -1.824, -2.038, -1.950, -1.970
Atom 15, -5.728, -3.420, -3.556, -3.849, -2.145, -2.174, -1.843, -2.155, -2.047, -2.223
Atom 16, -5.728, -3.391, -3.547, -3.839, -2.145, -2.174, -1.843, -2.145, -2.047, -2.213
Atom 17, -4.296, -3.099, -3.303, -2.534, -1.950, -1.434, -1.512, -1.921, -1.648, -1.785
Atom 18, -5.582, -3.722, -3.722, -3.479, -2.184, -1.415, -1.765, -2.057, -1.989, -1.999
Atom 19, -7.967, -4.540, -4.793, -4.550, -3.547, -3.079, -4.063, -7.295, -5.513, -5.455
Atom 20, -7.996, -4.569, -4.842, -4.579, -3.508, -3.060, -4.034, -7.139, -5.533, -5.474
Atom 21, -4.219, -3.177, -3.216, -1.804, -1.940, -1.502, -1.512, -1.921, -1.639, -1.746
Atom 22, -4.219, -3.187, -3.216, -1.804, -1.940, -1.522, -1.522, -1.931, -1.658, -1.765
Atom 23, -4.209, -3.187, -3.206, -1.833, -1.940, -1.512, -1.512, -1.911, -1.629, -1.746
Atom 24, -4.209, -3.167, -3.206, -1.824, -1.940, -1.522, -1.522, -1.921, -1.648, -1.755
Atom 25, -4.199, -3.216, -3.216, -1.804, -1.940, -1.522, -1.512, -1.911, -1.639, -1.746
Atom 26, -4.209, -3.225, -3.216, -1.814, -1.940, -1.531, -1.522, -1.911, -1.648, -1.755

C_2 adsorbed on Ni_{12} cluster

Ni1	2.1580000030	1.2459199685	2.0345799900

Ni2	2.1579999864	3.7377600148	2.0345800062
Ni3	5.0353300080	1.2459199694	2.0345799964
Ni4	5.0353300108	3.7377600149	2.0345800027
Ni5	1.4200999963	-0.0045099874	4.0412900364
Ni6	5.8026900018	0.0045000115	4.0564100326
Ni7	1.4201000017	4.9791799968	4.0412900349
Ni8	5.8026899978	4.9881899962	4.0564100336
Ni9	1.4549901640	2.4932900027	4.2289899387
Ni10	3.6063099909	1.1736003571	4.0199199818
Ni11	3.6099800311	3.8075096326	4.0213400139
Ni12	5.7789898083	2.4860300228	4.2202299328
C13	4.2689734354	2.4821218172	5.5689291832
C14	2.9826708942	2.4903738041	5.5573492577

Thermochemical properties at 1.0000 atm
rotational symmetry number: 1
rotational temperatures (K): 0.000053 0.000050 0.000034
vibrational temperatures:

mode:	1	2	3	4	5	6
temp. (K):	16.82	21.90	22.56	25.68	27.97	28.42
mode:	7	8	9	10	11	12
temp. (K):	500.47	512.59	624.08	795.31	822.03	2570.44

Thermodynamic properties calculated assuming an ideal gas
In the table below, the uNits for temperature
are kelvins, the uNits for U, H, and G are
kcal/mol and the uNits for Cv and S are cal/(mol K)

The zero point energy (ZPE): 5.930 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	60.853	1.481	-16.662	28.12229
rot.	0.889	2.981	50.940	0.889	-14.299	24.13416
vib.	4.269	18.709	46.409	4.269	-9.568	16.14843
elec.	0.000	0.000	3.867	0.000	-1.153	1.94591
total	6.046	24.671	162.069	6.639	-41.682	70.35079

Total internal energy, Utot (SCFE + ZPE + U): -2107.888583 hartrees
Total enthalpy, Htot (Utot + pV): -2107.887639 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2107.964643 hartrees

C_2 gas in periodic cell

2 6.59280 4.98369 23.01920 90.00000 90.00000 90.00000

C 2.14719 1.27084 5.31342
C 1.91771 1.48106 6.58892

FINAL RELAXED ENERGY = -22.1424113199

C_2 gas in non-periodic calculation

C1	0.0000000000	0.0000000000	0.6552364939
C2	0.0000000000	0.0000000000	-0.6552364939

Thermochemical properties at 1.0000 atm
rotational symmetry number: 2
rotational temperatures (K): 2.353868 2.353868

vibrational temperatures:
mode: 1
temp. (K): 2450.06

Thermodynamic properties calculated assuming an ideal gas
In the table below, the units for temperature
are kelvins, the units for U, H, and G are
kcal/mol and the units for Cv and S are cal/(mol K)

The zero point energy (ZPE): 2.434 kcal/mol
is not included in U, H, or G in the table below

T = 298.15 K

	U	Cv	S	H	G	ln(Q)
trans.	0.889	2.981	35.464	1.481	-9.092	15.34620
rot.	0.592	1.987	10.231	0.592	-2.458	4.14839
vib.	0.001	0.036	0.005	0.001	0.000	0.00027
elec.	0.000	0.000	2.183	0.000	-0.651	1.09861
total	1.483	5.004	47.883	2.075	-12.201	20.59348

Total internal energy, Utot (SCFE + ZPE + U): -75.909464 hartrees
Total enthalpy, Htot (Utot + pV): -75.908520 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -75.931271 hartrees